Reyes 09/646,110

=> => fil lreg

FILE 'LREGISTRY' ENTERED AT 10:55:18 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

LREGISTRY IS A STATIC LEARNING FILE

=> fil beilstein

FILE 'BEILSTEIN' ENTERED AT 10:55:23 ON 03 JUN 2004 COPYRIGHT (c) 2004 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002 FILE LAST UPDATED ON MARCH 30,2004

FILE COVERS 1771 TO 2003. \*\*\* FILE CONTAINS 8,932,479 SUBSTANCES \*\*\*

separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/ $\bar{\text{FA}}$ . The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN).

>>> PLEASE NOTE: Reaction data and substance data are stored in

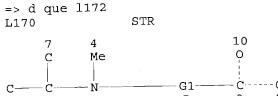
>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

searching RX.PBRNs or RX.RBRNs as BRNs. <<<

- \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* \* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.
- \* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE

After a search for reaction details substance documents associated with reactants or products may be retrieved by

- \* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE
- \* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.
- \* FOR PRICE INFORMATION SEE HELP COST \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*



```
REP G1 = (1-2) CH2
NODE ATTRIBUTES:
CONNECT IS E3 RC AT
CONNECT IS E3
              RC AT
CONNECT IS E1
              RC AT
                       6
CONNECT IS E1 RC AT
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

O SEA FILE=BEILSTEIN SSS FUL L170

=> d que 1175 STR L171 7 10 0 С Η ----O G1 C - N-8 1

REP G1=(1-2) CH2 NODE ATTRIBUTES:

CONNECT IS E2 RC AT CONNECT IS E3 RC AT 3 CONNECT IS E1 RC AT 6 CONNECT IS E1 RC AT DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

4 SEA FILE=BEILSTEIN SSS FUL L171 L173

1 SEA FILE=BEILSTEIN ABB=ON PLU=ON L173 NOT RN/FA L1741 SEA FILE=BEILSTEIN ABB=ON PLU=ON L174 AND PY<1999 L175

=> d 1175 ide

L175 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):

7957992

Chemical Name (CN):

Autonom Name (AUN):

3-isopropylamino-propionic acid; compound

with trifluoro-acetic acid

3-isopropylamino-propionic acid; compound

with trifluoro-acetic acid C6 H13 N O2 , C2 H F3 O2

Fragm. Molec. Formula (FMF):

C6 H13 N O2 . C2 H F3 O2 131.17, 114.02

Molecular Formula (MF): Molecular Weight (MW):

3043934, 742035 3388, 2836, 1157

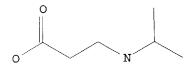
Fragment BRN (FBRN): Lawson Number (LN):

# Reyes 09/646,110

Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 6821411
Tautomer ID (TAUTID): 7567547
Beilstein Citation (BSO): 6-04
Entry Date (DED): 1998/11/09
Update Date (DUPD): 1998/11/09

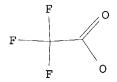
CM 1

FBRN 3043934 FMF C6 H13 N O2



CM 2

FBRN 742035 FMF C2 H F3 O2



# Field Availability:

Code	Name	Occurrence
=======	_======================================	========
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2 -
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	2

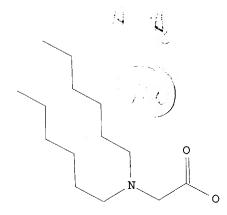
This substance also occurs in Reaction Documents:

Code Name Occurrence

```
RX
             Reaction Documents
              Substance is Reaction Product
    RXPRO
=> d l175 rx
L175 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN
Reaction:
RX
                                   4887359
    Reaction ID (.ID):
                                   635744, 605259
    Reactant BRN (.RBRN):
                                   acryloyl chloride, isopropylamine
    Reactant (.RCT):
                                   7957992
    Product BRN (.PBRN):
                                   3-isopropylamino-propionic acid; compound
    Product (.PRO):
                                   with trifluoro-acetic acid
    No. of React. Details (.NVAR):
Reaction Details:
RX
                                   4887359.1
    Reaction RID (.RID):
    Reaction Classification (.CL): Preparation
                                   Yield given. Multistep reaction
    Note(s) (.COM):
    Reference(s):
    1. Hamper, Bruce C.; Kolodziej, Stephen A.; Scates, Angela M.; Smith,
       Ronald G.; Cortez, Enriqueta, J.Org.Chem., CODEN: JOCEAH, 63(3),
        <1998>, 708-718; BABS-6090109
=> d que 1185
               STR
L182
    10
     0
                          — CH2—— CH2—— CH2—— CH2—— CH3
                      -N-
                                                           13
                                                     12
                                6
                                        8
                                              11
                           3
         5
                      ٦
REP G1 = (1-2) CH2
NODE ATTRIBUTES:
CONNECT IS E3 RC AT
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12
STEREO ATTRIBUTES: NONE
             5 SEA FILE=BEILSTEIN SSS FUL L182
L183
              2 SEA FILE=BEILSTEIN ABB=ON PLU=ON L183 NOT RN/FA
L184
              2 SEA FILE=BEILSTEIN ABB=ON PLU=ON L184 AND PY<1999
L185
=> d 1185 ide 1
```

L185 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

```
7917164
Beilstein Records (BRN):
Chemical Name (CN):
                               dihexylamino-acetic acid
                               dihexylamino-acetic acid
Autonom Name (AUN):
                               C14 H29 N O2
Molec. Formula (MF):
                               243.39
Molecular Weight (MW):
                               3379, 2862
Lawson Number (LN):
Compound Type (CTYPE):
                               acyclic
Constitution ID (CONSID):
                               6761800
                               7498208
Tautomer ID (TAUTID):
                               6-04
Beilstein Citation (BSO):
                               1998/11/09
Entry Date (DED):
                               1998/11/09
Update Date (DUPD):
```



# Field Availability:

Code	Name	Occurrence
========	=======================================	========
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1

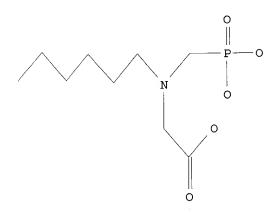
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=======	:======================================	========
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d 1185 ide 2

# L185 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 2271280 Hexyl-N-phosphonomethylglycinat Chemical Name (CN): (hexyl-phosphonomethyl-amino) -acetic acid Autonom Name (AUN): C9 H20 N O5 P Molec. Formula (MF): Molecular Weight (MW): 253.23 Lawson Number (LN): Compound Type (CTYPE): 3379, 2862, 689 acyclic 2090128 Constitution ID (CONSID): 2195791 Tautomer ID (TAUTID): Beilstein Citation (BSO): 5-04 Entry Date (DED): 1989/06/29 1992/06/02 Update Date (DUPD):



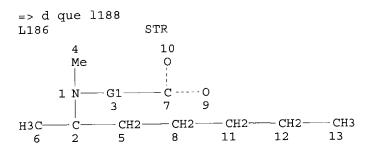
# Field Availability:

Code	Name	Occurrence
=======	=======================================	=======================================
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence

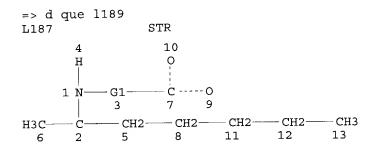
RX Reaction Documents
RXPRO Substance is Reaction Product



REP G1=(1-2) CH2
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 1
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE L188 0 SEA FILE=BEILSTEIN SSS FUL L186



REP G1=(1-2) CH2
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 1
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE L189 0 SEA FILE=BEILSTEIN SSS FUL L187

=>

4/45

# Reyes 09/646,110

06/03/2004

# => fil zcaplus

FILE 'ZCAPLUS' ENTERED AT 08:51:52 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

### => fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:51:55 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### => fil biosis

FILE 'BIOSIS' ENTERED AT 08:51:59 ON 03 JUN 2004 COPYRIGHT (C) 2004 BIOLOGICAL ABSTRACTS INC.(R)

FILE COVERS 1969 TO DATE. CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 2 June 2004 (20040602/ED)

FILE RELOADED: 19 October 2003.

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:52:02 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 1153 1) SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND L98 ( DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?) /AU L99 SEL PLU=ON L98 1 RN : 103 TERMS L100( 103) SEA FILE=REGISTRY ABB=ON PLU=ON L99 L101 SCR 1518 L102SCR 2050 2052 2043 L103 SCR 1526 L104 SCR 1235 L105 STR 8 CH\rightarrow CH3 CH\sigma Et H3C√√C√√CH3

8
2 G4 4
CH CH3
CH Et H3C C CH3
1 Ak
N
C
O
7

H3C~~ C~~ Et 16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
VAR G4=H/CH3
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

```
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18
```

```
STEREO ATTRIBUTES: NONE
1.106
               SCR 963
L107(
        3584468) SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)
               OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)
            526) SEA FILE=REGISTRY SUB=L107 SSS FUL ((L101 AND L103 AND L104
               AND L106) NOT L102) AND L105
L109(
             37) SEA FILE=REGISTRY ABB=ON PLU=ON L100 NOT (?NITRILE? OR
                ?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS
              2) SEA FILE=REGISTRY ABB=ON PLU=ON L108 AND (C6 H13 N O2) /MF
L110(
               AND (?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS
             39)SEA FILE=REGISTRY ABB=ON PLU=ON L110 OR L109
L111(
L112(
             16) SEA FILE=REGISTRY ABB=ON PLU=ON (16217-35-9/CRN OR 244189-98-
                8/CRN OR 244189-99-9/CRN OR 244190-00-9/CRN OR 244190-01-0/CRN
               OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR
               27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/
               CRN OR 41331-10-6/CRN OR 42313-51-9/CRN)
            41) SEA FILE=REGISTRY ABB=ON PLU=ON L111 OR L112
L113 (
L114 (
            18) SEA FILE=HCAPLUS ABB=ON PLU=ON L113 (L) (BIOL OR USES) /RL
L115 (
            14) SEA FILE=HCAPLUS ABB=ON PLU=ON L114 AND (PY<1999 OR AY<1999
               OR PRY<1999)
             3) SEA FILE=HCAPLUS ABB=ON PLU=ON L115 NOT (PESTICIDE? OR
L116(
               PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR UNIT? OR
               NONCONDENSED?)/SC
L117(
             4) SEA FILE=HCAPLUS ABB=ON PLU=ON L114 NOT L115
            43) SEA FILE=HCAPLUS ABB=ON PLU=ON L113 (L) PREP/RL
L118(
            40) SEA FILE=HCAPLUS ABB=ON PLU=ON L118 AND (PY<1999 OR AY<1999
L119(
               OR PRY<1999)
            22) SEA FILE=HCAPLUS ABB=ON PLU=ON L119 AND PATENT/DT
L120(
L121(
            10) SEA FILE=HCAPLUS ABB=ON PLU=ON L120 AND US/PC.B
L122
               STR
        8
                         CH3<sub>4</sub>
                                     <sub>5</sub>0<sup>6</sup>
                                                13 @14 15
```

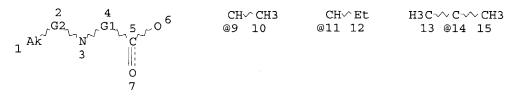
H3C-\(\sim C-\sim Et\)
16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E3 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE L123 STR



H3C~~C~~Et 16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E2 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

DILIKEO	ATTRIDOT										
L124 (	295	) SEA	FILE=REGISTR	Y SUB=L1	08 SSS F1	UL (L12	22 C	R L123)			
								(BIOL OR USES)/RL			
L126 (	480	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L125 A	MAND	(PY<1999 OR AY<1999			
		OR :	PRY<1999)								
L127(	389	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L126 A	MD	PATENT/DT			
L128(	67	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L127 A	AND	US/PC.B			
L129(	25	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L128 N	TOV	(UNIT? OR LEATHER?			
		OR I	DETERGENT? OR	PHOTOGRA	APHIC? O	R FOSSI	IL?	OR INK? OR ALLOY? OR			
EXPLOSIVE? OR PESTICID? OR WOOD? OR PETROLEUM? OR INORGANIC?											
			PLASTIC?)/SC								
L130(	25	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L129 N	TON	((L116 OR L117))			
			FILE=HCAPLUS			L130 N	TON	(AGRO?)/SC			
L132(	12	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L131 A	AND	(COSMET?)/SC			
L133 (	12	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L131 N	TON	L132			
L134(	126	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L124 (	(L)	PREP/RL			
L135(	106	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L134 A	AND	(PY<1999 OR AY<1999			
		OR I	PRY<1999)								
L136(	52	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L135 A	ND	PATENT/DT			
L137(	10	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L136 A	ND	US/PC.B			
L138(	5	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L137 N	TOI	L121			
L139(	10	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L121 N	TO	L116			
L140(	12	) SEA	FILE=HCAPLUS	ABB=ON	PLU≃ON	L133 N	TO	L116			
L141(	4	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L138 N	TOI	(L116 OR L133)			
L142(	55	) SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	"DYCK	L E	"/AU OR ("DYCK			
								LILLIAN E"/AU OR			
			CK LILLIAN EVA					·			
L143(	184				PLU=ON	DAVIS/	/AU	OR ("DAVIS B"/AU OR			

	"DAVIS B A"/AU)
L144 (	1591)SEA FILE=HCAPLUS ABB=ON PLU=ON "LIU Y"/AU OR "LIU Y D"/AU OR "LIU YA DONG"/AU
L145(	80)SEA FILE=HCAPLUS ABB=ON PLU=ON ("DURDEN D"/AU OR "DURDEN D
,	A"/AU) OR ("DURDEN DAVE A"/AU OR "DURDEN DAVID"/AU OR "DURDEN
	DAVID A"/AU)
L146(	341)SEA FILE=HCAPLUS ABB=ON PLU=ON ("BOULTON A"/AU OR "BOULTON A
	A"/AU) OR ("BOULTON ALAN"/AU OR "BOULTON ALAN A"/AU)
L147(	4) SEA FILE=HCAPLUS ABB=ON PLU=ON PETERSON/AU OR ("PETERSON
	I"/AU OR "PETERSON I ALICK"/AU)
L148(	527)SEA FILE=HCAPLUS ABB=ON PLU=ON KENNEDY/AU OR ("KENNEDY B"/AU
	OR "KENNEDY B A"/AU OR "KENNEDY B C"/AU OR "KENNEDY B F"/AU OR
	"KENNEDY B G"/AU OR "KENNEDY B H"/AU OR "KENNEDY B J"/AU OR
	"KENNEDY B L"/AU OR "KENNEDY B M"/AU OR "KENNEDY B MACK"/AU OR
	"KENNEDY B P"/AU OR "KENNEDY B P C"/AU OR "KENNEDY B R"/AU OR
	"KENNEDY B S"/AU OR "KENNEDY B W"/AU) OR ("KENNEDY BRENDA
	J"/AU OR "KENNEDY BRENDA SCHAFER"/AU OR "KENNEDY BRENDA V"/AU)
L149(	
	A"/AU OR "ROGERS K B"/AU OR "ROGERS K C"/AU OR "ROGERS K D"/AU
	OR "ROGERS K E"/AU OR "ROGERS K F"/AU OR "ROGERS K H"/AU OR
	"ROGERS K J"/AU OR "ROGERS K L"/AU OR "ROGERS K M"/AU OR
	"ROGERS K N"/AU OR "ROGERS K R"/AU OR "ROGERS K S"/AU OR
	"ROGERS K T"/AU OR "ROGERS K V"/AU OR "ROGERS K W"/AU) OR
	("ROGERS KEVIN"/AU OR "ROGERS KEVIN B"/AU OR "ROGERS KEVIN
	BONZI"/AU OR "ROGERS KEVIN J"/AU OR "ROGERS KEVIN M"/AU OR
	"ROGERS KEVIN P"/AU OR "ROGERS KEVIN PHILIP"/AU OR "ROGERS
	KEVIN PHILLIP"/AU OR "ROGERS KEVIN R"/AU)
L150(	2900) SEA FILE=HCAPLUS ABB=ON PLU=ON (L142 OR L143 OR L144 OR L145
	OR L146 OR L147 OR L148 OR L149)
L151(	1552) SEA FILE=HCAPLUS ABB=ON PLU=ON L150 AND (PY<1999 OR PRY<1999
/	OR AY<1999)
L152(	4)SEA FILE=HCAPLUS ABB=ON PLU=ON L151 AND (?SASKATCHEWAN?)/SO,P A
L153	3 SEA FILE=HCAPLUS ABB=ON PLU=ON L152 NOT (L116 OR L139 OR
	L140 OR L141)

=> s 1153 not (138 or 197) L168 3 L153 NOT (L38 OR L97)

# => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:52:43 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: May 28, 2004 (20040528/UP).

d que 1167

L154( 79)SEA FILE=BIOSIS ABB=ON PLU=ON "DYCK L"/AU OR "DYCK L E"/AU
OR ("DYCK LILLIAN"/AU OR "DYCK LILLIAN E"/AU)

L155( 553)SEA FILE=BIOSIS ABB=ON PLU=ON DAVIS/AU OR ("DAVIS B"/AU OR

"DAVIS B A"/AU) OR ("DAVIS BRUCE"/AU OR "DAVIS BRUCE A"/AU)

L156(

3449)SEA FILE=BIOSIS ABB=ON PLU=ON LIU/AU OR ("LIU Y"/AU OR "LIU
Y A"/AU OR "LIU Y B"/AU OR "LIU Y C"/AU OR "LIU Y C L"/AU OR
"LIU Y D"/AU OR "LIU Y DIANA"/AU OR "LIU Y E"/AU OR "LIU Y
F"/AU OR "LIU Y FANG"/AU OR "LIU Y G"/AU OR "LIU Y H"/AU OR
"LIU Y I"/AU OR "LIU Y J"/AU OR "LIU Y K"/AU OR "LIU Y LUCY"/AU OR "LIU Y M"/AU OR "LIU Y N"/AU OR "LIU Y N

```
C"/AU OR "LIU Y O"/AU OR "LIU Y P"/AU OR "LIU Y O"/AU OR "LIU
                Y O E"/AU OR "LIU Y R"/AU OR "LIU Y S"/AU OR "LIU Y S V"/AU OR
                "LIU Y SHIUAN"/AU OR "LIU Y SR"/AU OR "LIU Y T"/AU OR "LIU Y
                W"/AU OR "LIU Y X"/AU OR "LIU Y Y"/AU OR "LIU Y YI"/AU OR "LIU
                Y YONG"/AU OR "LIU Y YU"/AU OR "LIU Y Z"/AU OR "LIU Y ZHEN"/AU
                OR "LIU YA"/AU) OR "LIU YA DONG"/AU
             81) SEA FILE=BIOSIS ABB=ON PLU=ON ("DURDEN D"/AU OR "DURDEN D
L157(
                A"/AU) OR ("DURDEN DAVID"/AU OR "DURDEN DAVID A"/AU)
            390) SEA FILE-BIOSIS ABB-ON PLU-ON ("BOULTON A"/AU OR "BOULTON A
L158(
                A"/AU) OR ("BOULTON ALAN"/AU OR "BOULTON ALAN A"/AU)
             13) SEA FILE=BIOSIS ABB=ON PLU=ON ("PETERSON I"/AU OR "PETERSON
L159(
                I A"/AU) OR "PETERSON IAN"/AU
            839) SEA FILE-BIOSIS ABB-ON PLU-ON KENNEDY/AU OR ("KENNEDY B"/AU
L160(
                OR "KENNEDY B B"/AU OR "KENNEDY B C"/AU OR "KENNEDY B D"/AU OR
                "KENNEDY B E"/AU OR "KENNEDY B F"/AU OR "KENNEDY B G"/AU OR
                "KENNEDY B H"/AU OR "KENNEDY B J"/AU OR "KENNEDY B K"/AU OR
                "KENNEDY B L"/AU OR "KENNEDY B M"/AU OR "KENNEDY B N"/AU OR
                "KENNEDY B P"/AU OR "KENNEDY B P C"/AU OR "KENNEDY B R"/AU OR
                "KENNEDY B R C"/AU OR "KENNEDY B S"/AU OR "KENNEDY B V"/AU OR
                "KENNEDY B W"/AU) OR "KENNEDY BRENDA"/AU
L161(
            609) SEA FILE=BIOSIS ABB=ON PLU=ON ("ROGERS K"/AU OR "ROGERS K
               A"/AU OR "ROGERS K B"/AU OR "ROGERS K C"/AU OR "ROGERS K D"/AU
                OR "ROGERS K E"/AU OR "ROGERS K F"/AU OR "ROGERS K G"/AU OR
                "ROGERS K H"/AU OR "ROGERS K J"/AU OR "ROGERS K K"/AU OR
                "ROGERS K L"/AU OR "ROGERS K M"/AU OR "ROGERS K P"/AU OR
                "ROGERS K R"/AU OR "ROGERS K S"/AU OR "ROGERS K T"/AU OR
                "ROGERS K V"/AU OR "ROGERS K W"/AU) OR ("ROGERS KEVIN"/AU OR
                "ROGERS KEVIN B"/AU OR "ROGERS KEVIN H"/AU OR "ROGERS KEVIN
                L"/AU OR "ROGERS KEVIN M"/AU OR "ROGERS KEVIN R"/AU)
L162(
           5836) SEA FILE=BIOSIS ABB=ON PLU=ON (L154 OR L155 OR L156 OR L157
               OR L158 OR L159 OR L160 OR L161)
          4685) SEA FILE=BIOSIS ABB=ON PLU=ON L162 AND (PY<1999 OR MY<1999)
L163(
           163) SEA FILE=BIOSIS ABB=ON PLU=ON L163 AND ?SASKATCHEWAN?/CS.SO
L164(
              8) SEA FILE=BIOSIS ABB=ON PLU=ON L164 AND (?APOPTO? OR ANTIAPOPT
L165(
               02)
             3) SEA FILE=BIOSIS ABB=ON PLU=ON L164 AND (?CELL? (5A) (?RESCU?
L166(
               OR ?DEATH?))
            11 SEA FILE=BIOSIS ABB=ON PLU=ON L165 OR L166
L167
```

=> dup rem 1168 1167

FILE 'HCAPLUS' ENTERED AT 08:52:53 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'BIOSIS' ENTERED AT 08:52:53 ON 03 JUN 2004
COPYRIGHT (C) 2004 BIOLOGICAL ABSTRACTS INC.(R)
PROCESSING COMPLETED FOR L168
PROCESSING COMPLETED FOR L167
L169 13 DUP REM L168 L167 (1 DUPLICATE REMOVED)

ANSWERS '1-3' FROM FILE HCAPLUS ANSWERS '4-13' FROM FILE BIOSIS

=>

=>

### => d 1169 ibib abs 1-3

L169 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1

ACCESSION NUMBER:

1998:774327 HCAPLUS

DOCUMENT NUMBER:

129:343272

TITLE:

Preparation of aliphatic propargylamines as

neuroprotective agents

INVENTOR(S):

Durden, David; Paterson, Alick; Davis,

Bruce; Dyck, Lillian; Yu, Peter; Li, Xinmin;

Boulton, Alan

PATENT ASSIGNEE(S):

University of Saskatchewan, Can.

SOURCE:

U.S., 12 pp.

DOCUMENT TYPE:

CODEN: USXXAM

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	NO.		KI	ND	DATE			A	PPLI	CATI	ON NC	ο.	DATE			
US 584 US 625 WO 990 WO 990	1950 3817		A B A	1 2	1998: <del>2001</del> : 1999: 1999:	0626 0128		U	S 19	 97-8 98-1 98-C	1054	8	1997 1998 1998	0706	<	Λ
W:	KP, NO, UA, : GH, FI,	EE, KR, NZ, UG, GM, FR,	ES, KZ, PL, US, KE, GB,	FI, LC, PT, UZ, LS, GR,	GB, LK, RO, VN, MW,	GE, LR, RU, YU, SD, IT,	GH, LS, SD, ZW, SZ, LU,	GM, LT, SE, AM, UG, MC,	HR, LU, SG, AZ, ZW, NL,	HU, LV, SI, BY, AT, PT,	ID, MD, SK, KG, BE,	IL, MG, SL, KZ, CH,	CN, IS, MK, TJ, MD, CY, BJ,	JP, MN, TM, RU, DE,	KE, MW, TR, TJ, DK,	KG, MX, TT, TM ES,
AU 988 EP 996					1999) 2000)					98-8: 98-9:			19980 19980		-	
EP 996 R:	612 DE,	FR,	B: GB,	_	2003	0409										

PRIORITY APPLN. INFO.:

JP 2001510179 T2 20010731

OTHER SOURCE(S):

MARPAT 129:343272

AB Aliphatic propargylamines HC.tplbond.CCH2NHCH(R1)R2 [R1 = H, CH3; R2 = CH3(CH2)n; n = 0-16; such that if R1 = H then n >4, if R1 = CH3 then n ≠ 0, and if R1 = CH3 and n = 1-4 then the title compound is in the form of a pure enantiomer in the (R)-configuration] and their salts, useful as neuroprotective and anti-ischemic agents in the treatment and prevention of cell death by apoptosis, are prepared Thus, (R)-2-heptylamine (prepared by the resolution of 2-heptylamine) was condensed with propargyl bromide and salified with HCl, producing (R)-N-2-heptylpropargylamine hydrochloride which demonstrated a 230 ± 36% (at 0.1 mg/kg, p.o.) survival in a rat model of apoptosis of hippocampal pyramidal neurons by hypoxia/ischemia, vs. 100 ± 22% survival for water.

WO 1998-CA683

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

JP 2000-503049 19980714 <--

W 19980714 <--

US 1997-891904 A3 19970714 <--

L169 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:468566 HCAPLUS

DOCUMENT NUMBER:

131:111423

TITLE:

Composition containing a propargylamine for enhancing

cancer therapy

INVENTOR(S):

Paterson, I. Alick; Boulton, Alan A.

NIAL

PATENT ASSIGNEE(S):

University of Saskatchewan Technologies

Inc., Can.; The Canada Trust Company; Warrington, R.

SOURCE:

PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

```
PATENT NO.
                    KIND DATE
                                        APPLICATION NO. DATE
                         -----
    WO 9936076 A1 19990722
                                      WO 1999-CA5 19990113 <--
        W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
            DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
            KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
            MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
            TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU.
            TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
            CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    CA 2318693
                     AA 19990722
                                        CA 1999-2318693 19990113 <--
    AU 9919563
                     A1
                          19990802
                                        AU 1999-19563
                                                        19990113 <--
    EP 1049478
                     Α1
                          20001108
                                        EP 1999-900405
                                                       19990113 <--
    EP 1049478
                     В1
                          20020904
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, FI
    AT 223209
                          20020915
                                        AT 1999-900405
                                                        19990113 <--
    HK 1032204
                          20030509
                                       HK 2001-102511
                    A1
                                                        20010410 <--
                                     US 1998-71023P P 19980113 <--
PRIORITY APPLN. INFO.:
                                     WO 1999-CA5
                                                    W 19990113
```

OTHER SOURCE(S): MARPAT 131:111423

Antineoplastic drug modulators are described. The specific modulators referred to are propargylamines which can enhance the cytotoxic effects of antineoplastic drugs on cancer cells while protecting normal cells from damage. The propargylamine modulators can be used to increase the selectivity and effectiveness of conventional antineoplastic drugs, to reduce the unwanted side-effects of cancer chemotherapy, to improve effectiveness of cancer chemotherapy, to improve treatment of cancers for which treatment is otherwise ineffective, to improve therapy of cancers otherwise unresponsive or poorly responsive due to drug-resistance and/or toxicity limited treatment regimens and to render effective chemotherapy for previously untreatable cancers.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS 2 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L169 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:59281 HCAPLUS

DOCUMENT NUMBER:

118:59281

TITLE:

Preparation of aliphatic propargylamines as selective

MAO-B inhibitors and neuroprotective agents Yu, Peter H.; Davis, Bruce A.; Boulton, Alan

PATENT ASSIGNEE(S):

University of Saskatchewan, Can.

SOURCE:

PCT Int. Appl., 81 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

LANGUAGE:

INVENTOR(S):

Patent English

FAMILY ACC. NUM. COUNT: 1

### PATENT INFORMATION:

```
KIND DATE
    PATENT NO.
                                         APPLICATION NO. DATE
                     ____ /____
    WO 9215551
                    A1 19920917
                                         WO 1992-CA90
                                                          19920228 <--
        W: AT, AU, BB, BG, BR, CA, CA, CS, DE, DK, ES, FI, GB, HU, JP, KP,
            KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US
        RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN,
            GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG
    US 5169868
                           19921208
                                         US 1991-663018
                                                          19910301 <--
                      Α
                           19921006
                                         AU 1992-13236
    AU 9213236
                      Α1
                                                          19920228 <--
    AU 658611
                           19950427
                      В2
    EP 573498
                                         EP 1992-905512
                           19931215
                                                          19920228 <--
                      A1
    EP 573498
                           19981118
                      _{\rm B1}
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE
                                         JP 1992-504826
    JP 06505241
                     T2
                           19940616
                                                         19920228 <--
    JP 3129733
                      B2
                           20010131
    AT 173459
                                         AT 1992-905512
                      E
                           19981215
                                                          19920228 <--
                                         US 1993-108653
    US 5508311
                           19960416
                                                          19931223 <--
                      Α
                                         HK 1998-115865 19981228 <--
    HK 1014533
                           20000505
                      Α1
PRIORITY APPLN. INFO.:
                                       US 1991-663018 A2 19910301 <--
                                       US 1991-633018 A 19910301 <--
                                                      A 19920228 <--
                                       WO 1992-CA90
                        MARPAT 118:59281
OTHER SOURCE(S):
```

R2CHR1NMeCH2C.tplbond.CH (I; R1 = H, alkyl; R2 = (substituted) C3-11 alkyl, -alkenyl, -alkynyl, -alkynyl, -alkoxy, -alkylthio, -alkylsulfinyl; with provisos), are prepared Me(CH2)2CH2Br, CH.tplbond.CCH2NHMe and anhydrous Na2CO3 were heated for 72 h in EtOH to give I (R1 = H, R2 = Pr).HCl (II). II inhibited MAO-B activity in mouse brain with ID50 = 2 mg/kg i.p.

=> d l169 ibib ab 4-YOU HAVE REQUESTED DATA FROM 10 ANSWERS - CONTINUE? Y/(N):y

L169 ANSWER 4 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

1998:124820 BIOSIS ACCESSION NUMBER: DOCUMENT NUMBER: PREV199800124820

R-Deprenyl and R-2-Heptyl-N-methylpropargylamine prevent TITLE:

apoptosis in cerebellar granule neurons induced by

cytosine arabinoside but not low extracellular potassium.

Paterson, I. A. [Reprint author]; Zhang, D.; Warrington, R. AUTHOR (S):

C.; Boulton, A. A.

Neuropsychiatry Res. Unit, Dep. Psychiatry, Al14 Med. Res. CORPORATE SOURCE:

Build., Univ. Saskatchewan, 103 Wiggins Road,

Saskatoon, Saskatchewan S7N 5E4, Canada

Journal of Neurochemistry, (Feb., 1998) Vol. 70, No. 2, pp. SOURCE:

515-523. print.

CODEN: JONRA9. ISSN: 0022-3042.

DOCUMENT TYPE: Article LANGUAGE: English

ENTRY DATE: Entered STN: 5 Mar 1998

Last Updated on STN: 5 Mar 1998

R-Deprenyl and R-2-heptyl-N-methylpropargylamine (R-2-HMP) are compounds AB that have been shown to reduce neuronal death in various in vitro and in vivo models involving apoptosis but do not always prevent apoptosis. In the present study we have examined the effects of these compounds and their S enantiomers on cytosine arabinoside (ara C) -induced apoptosis and low K+-induced apoptosis in cerebellar granule cells in primary culture. It was found that R-deprenyl and R-2-HMP could prevent ara C-induced apoptosis with an EC50

around 10-9 M but could not prevent low K+-induced apoptosis. S-Deprenyl and S-2-HMP did not prevent apoptosis under any conditions but were found to antagonize the antiapoptotic actions of R-deprenyl and R-2-HMP. Using the fluorescent mitochondrial dye chloromethyltetramethylrhodamine methyl ester it was found that there was a loss of mitochondrial function in cerebellar granule cells exposed to ara C but not low K+ medium. R-Deprenyl and R-2-HMP prevented the ara C-induced loss of mitochondrial function. It is concluded that R-deprenyl and R-2-HMP prevent apoptosis of cerebellar granule cells by a mechanism that is independent of monoamine oxidase inhibition and that they act on the same site to prevent specifically  ${\bf apoptosis}$ involving a loss of mitochondrial membrane potential, possibly p53-dependent apoptosis.

L169 ANSWER 5 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1999:283898 BIOSIS PREV199900283898

TITLE:

L-deprenyl induces aromatic L-amino acid decarboxylase

(AADC) mRNA in the rat substantia nigra and ventral

tegmentum: An in situ hybridization study.

AUTHOR(S):

Li, Xin-Min [Reprint author]; Juorio, Augusto V.; Qi, Jin;

Boulton, Alan A.

CORPORATE SOURCE:

Neuropsychiatry Research Unit, Department of Psychiatry,

University of Saskatchewan, Saskatoon, SK, S7N

5E4, Canada

SOURCE:

Molecular and Chemical Neuropathology, (Aug.-Dec., 1998)

Vol. 35, No. 1-3, pp. 149-155. print.

ISSN: 1044-7393.

DOCUMENT TYPE:

Article English

LANGUAGE: ENTRY DATE:

Entered STN: 28 Jul 1999

Last Updated on STN: 28 Jul 1999

L-Deprenyl is a complex drug, and number of mechanisms have been proposed AB to explain its effects. These include blockade of dopamine metabolism, amplification of dopamine responses, induction of superoxide dismutase or delaying apoptosis. Using in situ hybridization techniques, we have shown that L-deprenyl (5-10 mg/kg intraperitoneally, killed after 24 h) increases aromatic L-amino acid decarboxylase (AADC) mRNA levels in rat substantia nigraventral tegmental area. In human brain tissue, AADC is present at low levels, suggesting a possible rate-limiting role in monoamine synthesis. This is particularly important in parkinsonian patients, since the therapeutic efficacy of L-DOPA is attributed to its enzymatic decarboxylation to dopamine. The present findings support that one of the effects of L-deprenyl may be to facilitate the decarboxylation of L-DOPA by increasing the availability, of AADC.

L169 ANSWER 6 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1998:26851 BIOSIS PREV199800026851

TITLE:

Aliphatic N-methylpropargylamines: Monoamine oxidase-B inhibitors and antiapoptotic drugs.

AUTHOR (S):

Boulton, Alan A.; Yu, Peter H.; Davis, Bruce

A.; Paterson, I. Alick; Li, Xi-Min; Juorio, Augusto

V.; Durden, David A.; Dyck, Lillian E.

CORPORATE SOURCE:

Neuropsychiatry Res. Unit, Univ. Saskatchewan,

Saskatoon, SK S7N 5E4, Canada SOURCE:

Goldstein, D. S. [Editor]; Eisenhofer, G. [Editor] McCarty, R. [Editor]. Adv. Pharmacol. (San Diego),

pp. 308-311. Advances in Pharmacology; Catecholamines:

Bridging basic science with clinical medicine. print.

Page 10

Publisher: Academic Press, Inc., 1250 Sixth Ave., San Diego, California 92101, USA; Academic Press Ltd., 14 Belgrave Square, 24-28 Oval Road, London NW1 70X, England,

UK. Series: Advances in Pharmacology.

Meeting Info.: Eighth International Catecholamine

Symposium. Pacific Grove, California, USA. October 13-18,

1996.

CODEN: ADPHEL. ISSN: 1054-3589. ISBN: 0-12-032943-3.

DOCUMENT TYPE:

Book

Conference; (Meeting) Book; (Book Chapter)

Conference; (Meeting Paper)

LANGUAGE:

English

ENTRY DATE:

Entered STN: 5 Jan 1998

Last Updated on STN: 24 Feb 1998

L169 ANSWER 7 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1997:533932 BIOSIS PREV199799833135

TITLE:

The anti-apoptotic effects of 2HMP is due to a

desmethyl metabolite.

AUTHOR(S):

Paterson, I. A.; Dyck, L. E.; Durden, D.

A.; Davis, B. A.; Liu, Y.;

Boulton, A. A.

CORPORATE SOURCE:

Neuropsychiatry, Res. Unit, Dep. Psychiatry, Univ.

Saskatchewan, Saskatoon, SK S7N 5E4, Canada

SOURCE:

Society for Neuroscience Abstracts, (1997) Vol. 23, No.

1-2, pp. 2254.

Meeting Info.: 27th Annual Meeting of the Society for Neuroscience. New Orleans, Louisiana, USA. October 25-30,

1997.

ISSN: 0190-5295.

DOCUMENT TYPE:

Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

Conference; (Meeting Poster)

LANGUAGE:

English

ENTRY DATE:

Entered STN: 12 Dec 1997

Last Updated on STN: 12 Dec 1997

L169 ANSWER 8 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER:

1998:275926 BIOSIS

DOCUMENT NUMBER:

PREV199800275926

TITLE:

Alipathic propargylamines: New antiapoptotic

drugs.

AUTHOR(S):

Boulton, Alan A. [Reprint author]; Davis,

Bruce A.; Durden, David A.; Dyck,

Lillian E.; Juorio, Augusto V.; Li, Xin-Min; Paterson,

I. Alick; Yu, Peter H.

CORPORATE SOURCE:

Neuropsychiatry Res. Unit, A114 Med. Res. Build., Univ.

Saskatchewan, 103 Wiggins Road, Saskatoon, SK S7N

5E4, Canada

SOURCE:

Drug Development Research, (Nov.-Dec., 1997) Vol. 42, No.

3-4, pp. 150-156. print.

CODEN: DDREDK. ISSN: 0272-4391.

DOCUMENT TYPE:

Article

Ochera.

General Review; (Literature Review)

LANGUAGE:

English

ENTRY DATE:

Entered STN: 24 Jun 1998

Last Updated on STN: 13 Aug 1998

AB Two series of drugs, the aliphatic-N-methyl propargylamines and the

aliphatic propargylamines, have been synthesised and shown to be specific, irreversible, and potent monoamine oxidase B inhibitors and neural rescue agents. In the latter case, an absolute stereochemical requirement for the R isomer exists. Both series of compounds have been shown, in numerous in vitro and in vivo experimental paradigms, to be effective neuronal rescue agents. Candidates from both series exhibit excellent bioavailability and pharmacokinetics and offer opportunities for treating neurodegenerative disorders and stroke and cognitive decline in companion animals.

L169 ANSWER 9 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1997:382572 BIOSIS PREV199799681775

TITLE:

 $\hbox{$R$-deprenyl and $R$-2-heptylmethylpropargylamine prevent}$ 

P53-dependent but not P53-independent apoptosis. Paterson, I. A.; Warrington, R.; Boulton, A. A.

AUTHOR(S):
CORPORATE SOURCE:

Neuropsychiatry Res. Unit, Univ. Saskatchewan,

conforming booker.

103 Wiggins Road, Saskatoon, SK S7N 5E4, Canada

SOURCE: Journal of Neurochemistry, (1997) Vol. 69, No. SUPPL., pp. S137.

Meeting Info.: Joint Sixteenth Biennial Meeting of the International Society for Neurochemistry and Twenty-eighth Annual Meeting of the American Society for Neurochemistry.

Boston, Massachusetts, USA. July 20-26, 1997.

CODEN: JONRA9. ISSN: 0022-3/042.

DOCUMENT TYPE:

Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

LANGUAGE: English

ENTRY DATE:

Entered STN: 4 Sep 1997

Last Updated on STN: 4 Sep 1997

L169 ANSWER 10 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1996:527439 BIOSIS PREV199699249795

TITLE:

MK-801 induces apoptotic neuronal death in the

rat retrosplenial cortex: Prevention by cycloheximide and

R(-)-2-hexyl-N-methylpropargylamine.

AUTHOR (S):

Zhang, Xia; Boulton, Alan A.; Zuo, Dong-Mei; Yu,

Peter H. [Reprint author]

CORPORATE SOURCE:

Neuropsychiatry Res. Unit, Dep. psychiatry, Univ.

Saskatchewan, Saskatoon, Saskatchewan S7N

5E4, Canada

SOURCE:

Journal of Neuroscience Research, (1996) Vol. 46, No. 1,

pp. 82-89.

CODEN: JNREDK. ISSN: 0360-4012.

DOCUMENT TYPE:

Article

LANGUAGE:

English

ENTRY DATE:

Entered STN: 22 Nov 1996

Last Updated on STN: 23 Nov 1996

MK-801 is a non-competitive N-methyl-D-aspartate (NMDA) receptor antagonist which can prevent excitatory neuronal death. At higher concentrations, however, it can also induce neuronal death in the limbic system. This MK-801-induced selective neurotoxicity has been proposed as an animal model for dementia and psychosis. We have investigated the effects of the protein synthesis inhibitor cycloheximide and the neurorescue agent 2-hexyl-N-methylpropargylamine (R(-)-2HxMP) on MK-801-induced neuronal death in the retrosplenial cortex in the rat. Cycloheximide (2 mg/kg, subcutaneously (sc)) administered either 1 hr before, or after, injection of MK801 (5 mg/kg, sc) prevented almost completely neuronal shrinkage and nuclear condensation of the granular

retrosplenial cortex as assessed by hematoxylin-eosin staining. results suggest that the MK801-induced neuronal death was apoptotic. This neurorescue effect by cycloheximide was time dependent: after 4 hr the effect was reduced to about 50% and by 8 hr had disappeared. R(-)-2HxMP (0.25 mg/kg, sc), which does not inhibit protein synthesis in vitro, was also found to be effective at preventing MK-801-induced neuronal death.

L169 ANSWER 11 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1996:493093 BIOSIS PREV199699215449 DOCUMENT NUMBER:

TITLE: MK-801-induced expression of BCL-2, Fos and HSP72 proteins

in the rat cerebral cortex.

Zhang, X.; Fan, X.; Yu, P. H.; Boulton, A. A. AUTHOR(S): Neuropsychiatry Res. Unit, Dep. Psychiatry, Univ. CORPORATE SOURCE:

Saskatchewan, Saskatoon, SK S7N 5E4, Canada

Society for Neuroscience Abstracts, (1996) Vol. 22, No. SOURCE:

1-3, pp. 42.

Meeting Info.: 26th Annual Meeting of the Society for Neuroscience. Washington, D.C., USA. November 16-21, 1996.

ISSN: 0190-5295.

DOCUMENT TYPE: Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

Conference; (Meeting Poster)

LANGUAGE:

English

ENTRY DATE: Entered STN: 4 Nov 1996

Last Updated on STN: 5 Nov 1996

L169 ANSWER 12 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1995:147634 BIOSIS

PREV199598161934

TITLE: Neuroprotective effects of N-methylpropargylamines against

kainic acid induced neuronal damage in the rat brain.

Zhang, X.; Yu, P. H.; Davis, B. A.; Zuo, C. T.; AUTHOR(S):

Boulton, A. A.

Neuropsychiatry Res. Unit, Univ. Saskatchewan, CORPORATE SOURCE:

Saskatoon S7N 0W0, Canada

Journal of Neurochemistry, (1995) Vol. 64, No. SUPPL. 1, SOURCE:

pp. S96.

Meeting Info.: Twenty-sixth Meeting of the American Society for Neurochemistry. Santa Monica, California, USA. March

5-9, 1995.

CODEN: JONRA9. ISSN: 0022-3042.

DOCUMENT TYPE:

Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

LANGUAGE:

English

ENTRY DATE:

Entered STN: 3 Apr 1995

Last Updated on STN: 23 May 1995

L169 ANSWER 13 OF 13 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1994:535587 BIOSIS PREV199497548587

TITLE:

Neuroprotective effects of some monoamine oxidase-B

inhibitors against DSP-4-induced noradrenaline depletion in

the mouse hippocampus.

AUTHOR(S):

Yu, P. H. [Reprint author]; Davis, B. A.; Fang,

J.; Boulton, A. A.

CORPORATE SOURCE:

Neuropsychiatric Res. Unit, Dep. Psychiatry, Univ.

Saskatchewan, Saskatoon, SK S7N 0W0, Canada

SOURCE:

Journal of Neurochemistry, (1994) Vol. 63, No. 5, pp.

1820-1828.

CODEN: JONRA9. ISSN: 0022-3042.

DOCUMENT TYPE:

Article English

ENTRY DATE:

Entered STN: 15 Dec 1994

Last Updated on STN: 16 Dec 1994

DSP-4 (N-(2-chloroethyl)-N-ethyl-2-bromobenzylamine), a selective AΒ noradrenaline (NA) uptake blocker, is capable of inducing long-lasting depletion of NA in some noradrenergic axon terminals and of subsequently causing cell death to NA neuronal cell bodies in rodents. R(-)-Deprenyl, a selective monoamine oxidase (MAO)-B inhibitor, has been shown to be capable of protecting animals against this DSP-4-induced neuronal degeneration. Its action, however, has been claimed to be unrelated to the inhibition of MAO-B activity but rather due to competition for the NA uptake sites. The effects of several types of MAO inhibitors against DSP-4 toxicity, MAO-B activity both in vivo and in vitro, and NA uptake into the hippocampus have been assessed. N-(2-Hexyl) N-methylpropargylamine (2-HxMP), a potent MAO-B inhibitor, for example, exerts no appreciable effect on NA uptake but is quite potent in counteracting the NA-depleting effect of DSP-4. Such results rule out the possibility that the neuroprotective effect of the MAO-B inhibitors is due mainly to their effect on NA uptake. The in vitro inhibition of MAO-B activity seems to correlate positively with their neuroprotective effects against DSP-4. In comparison to the MAO-B inhibitors, NA uptake blockers, such as desipramine and S(+)-deprenyl, exhibit relatively low efficacy in protecting the NA axon terminals from the effects of DSP-4-induced damage. The restoration of hippocampal NA levels is significantly enhanced with repeated treatments of R(-)-deprenyl or 2-HxMP even at very low doses following the DSP-4 insult. This suggests that in addition to neuroprotection, these MAO-B inhibitors may rescue some of the noradrenergic axon terminals damaged by DSP-4.

### => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:54:15 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 28, 2004 (20040528/UP).

=>

### Reyes 09/646,110

06/03/2004

=> fil lreg

FILE 'LREGISTRY' ENTERED AT 08:45:30 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

LREGISTRY IS A STATIC LEARNING FILE

=> fil req

FILE 'REGISTRY' ENTERED AT 08:45:32 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1 DICTIONARY FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:45:36 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil zcaplus

FILE 'ZCAPLUS' ENTERED AT 08:45:44 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

# => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:45:48 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 28, 2004 (20040528/UP).

```
=> d que 196
              1) SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND
L39 (
                DYCK,L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?)/AU
                SEL PLU=ON L39 1 RN :
                                            103 TERMS
L40
            103) SEA FILE=REGISTRY ABB=ON PLU=ON L40
L41 (
                SCR 1518
1.42
                SCR 2050 2052 2043
L43
                SCR 1526
L44
L45
                SCR 1235
L46
                STR
```



H3C C Et 16 @17 18

REP G1=(1-3) CH2 VAR G2=CH2/9/11/14/17

```
VAR G4=H/CH3
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

**GRAPH ATTRIBUTES:** 

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

```
STEREO ATTRIBUTES: NONE
L47
                SCR 963
        3584468) SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)
L48 (
                OR (TIS OR MNS OR AYS OR PMS)/CI OR SEOUENCE/FS)
            526) SEA FILE=REGISTRY SUB=L48 SSS FUL ((L42 AND L44 AND L45 AND
L49 (
                L47) NOT L43) AND L46
             37) SEA FILE=REGISTRY ABB=ON PLU=ON L41 NOT (?NITRILE? OR
L50 (
                ?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS
              2) SEA FILE=REGISTRY ABB=ON PLU=ON L49 AND (C6 H13 N O2) /MF AND
L51 (
                (?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS
             39) SEA FILE=REGISTRY ABB=ON PLU=ON L51 OR L50
L52 (
             16) SEA FILE=REGISTRY ABB=ON PLU=ON (16217-35-9/CRN OR 244189-98-
L53 (
                8/CRN OR 244189-99-9/CRN OR 244190-00-9/CRN OR 244190-01-0/CRN
                OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR
                27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/
                CRN OR 41331-10-6/CRN OR 42313-51-9/CRN)
             41) SEA FILE=REGISTRY ABB=ON PLU=ON L52 OR L53
L54 (
             18) SEA FILE=HCAPLUS ABB=ON PLU=ON L54 (L) (BIOL OR USES)/RL
L55 (
             14) SEA FILE=HCAPLUS ABB=ON PLU=ON L55 AND (PY<1999 OR AY<1999
L56 (
                OR PRY<1999)
              3 SEA FILE=HCAPLUS ABB=ON PLU=ON L56 NOT (PESTICIDE? OR
L57
                PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR UNIT? OR
                NONCONDENSED?)/SC
              1) SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND
L58 (
                DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?) / AU
                SEL PLU=ON L58 1 RN: 103 TERMS
L59
            103) SEA FILE=REGISTRY ABB=ON PLU=ON L59
L60 (
                SCR 1518
L61
                SCR 2050 2052 2043
L62
                SCR 1526
L63
                SCR 1235
L64
L65
                STR
        8
        G4
                           CH\rightarrow CH3
                                      CH√ Et
                                                 H3C√√ C√√ CH3
                <sub>_</sub>0<sup>6</sup>
                                                   13 @14 15
                           @9 10
                                       @11 12
               0
```

H3C~~C~~Et

REP G1=(1-3) CH2 VAR G2=CH2/9/11/14/17 VAR G4=H/CH3

```
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

```
STEREO ATTRIBUTES: NONE
L66
                SCR 963
L67 (
        3584468) SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)
                OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)
L68 (
            526) SEA FILE=REGISTRY SUB=L67 SSS FUL ((L61 AND L63 AND L64 AND
                L66) NOT L62) AND L65
L69 (
             37) SEA FILE=REGISTRY ABB=ON PLU=ON L60 NOT (?NITRILE? OR
                ?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS
L70 (
              2) SEA FILE=REGISTRY ABB=ON PLU=ON L68 AND (C6 H13 N O2)/MF AND
                 (?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS
T<sub>1</sub>71 (
             39) SEA FILE=REGISTRY ABB=ON PLU=ON L70 OR L69
L72 (
             16) SEA FILE=REGISTRY ABB=ON PLU=ON (16217-35-9/CRN OR 244189-98-
                8/CRN OR 244189-99-9/CRN OR 244190-00-9/CRN OR 244190-01-0/CRN
                OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR
                27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/
                CRN OR 41331-10-6/CRN OR 42313-51-9/CRN)
             41) SEA FILE=REGISTRY ABB=ON PLU=ON L71 OR L72
L73 (
L74 (
             18) SEA FILE=HCAPLUS ABB=ON PLU=ON L73 (L) (BIOL OR USES)/RL
L75 (
             14) SEA FILE=HCAPLUS ABB=ON PLU=ON L74 AND (PY<1999 OR AY<1999
                OR PRY<1999)
L76 (
              3) SEA FILE=HCAPLUS ABB=ON PLU=ON L75 NOT (PESTICIDE? OR
                PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR UNIT? OR
                NONCONDENSED?)/SC
              4) SEA FILE=HCAPLUS ABB=ON PLU=ON L74 NOT L75
L77 (
L78
                STR
        CH3<sub>4</sub>
                            CH\rightarrow CH3
                                       CH√ Et
                                                  H3C-√ C-√ CH3
                 <sub>/</sub>0<sup>6</sup>
                           @9 10
                                        @11 12
                                                     13 @14 15
               0
         3
```

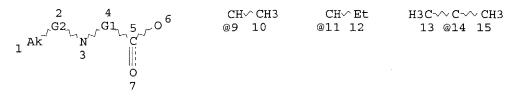
H3C-\(\sim C-\sim Et\)
16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E3 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE L79 STR



H3C~~C~~Et 16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E2 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:
PING(S) ARE ISOLATED O

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 17

NUMBER OF NODES 13 17

```
STEREO ATTRIBUTES: NONE
           295) SEA FILE=REGISTRY SUB=L68 SSS FUL (L78 OR L79)
L81 (
           598) SEA FILE=HCAPLUS ABB=ON PLU=ON L80 (L) (BIOL OR USES) /RL
L82 (
           480) SEA FILE=HCAPLUS ABB=ON PLU=ON L81 AND (PY<1999 OR AY<1999
               OR PRY<1999)
L83 (
           389) SEA FILE=HCAPLUS ABB=ON PLU=ON L82 AND PATENT/DT
            67) SEA FILE=HCAPLUS ABB=ON PLU=ON L83 AND US/PC.B
L84 (
L85 (
            25) SEA FILE=HCAPLUS ABB=ON PLU=ON L84 NOT (UNIT? OR LEATHER? OR
               DETERGENT? OR PHOTOGRAPHIC? OR FOSSIL? OR INK? OR ALLOY? OR
               EXPLOSIVE? OR PESTICID? OR WOOD? OR PETROLEUM? OR INORGANIC?
               OR PLASTIC?)/SC
            25) SEA FILE=HCAPLUS ABB=ON PLU=ON L85 NOT ((L76 OR L77))
L86 (
            24) SEA FILE=HCAPLUS ABB=ON PLU=ON L86 NOT (AGRO?)/SC
L87 (
            12) SEA FILE=HCAPLUS ABB=ON PLU=ON L87 AND (COSMET?)/SC
L88 (
           12) SEA FILE=HCAPLUS ABB=ON PLU=ON L87 NOT L88
           12 SEA FILE=HCAPLUS ABB=ON PLU=ON L89 NOT L76
            1 SEA FILE=REGISTRY ABB=ON PLU=ON 7631-98-3/RN
L91
           228 SEA FILE=HCAPLUS ABB=ON PLU=ON L91
L92
             4 SEA FILE=HCAPLUS ABB=ON PLU=ON L90 NOT L92
L93
L94
            8 SEA FILE=HCAPLUS ABB=ON PLU=ON L90 NOT L93
L95
            3 SEA FILE=HCAPLUS ABB=ON PLU=ON L94 AND (A61K?)/ICM
            10 SEA FILE=HCAPLUS ABB=ON PLU=ON L93 OR L57 OR L95
L96
```

=> d his 197

FILE 'HCAPLUS' ENTERED AT 08:07:49 ON 03 JUN 2004 L97 8 S L96 NOT L38

=> d 197 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L97 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:435212 HCAPLUS

DOCUMENT NUMBER:

139:3248

TITLE:

Betaines as adjuvants to susceptibility testing and

antimicrobial therapy

INVENTOR(S):

Thornton, Charles G. USA

PATENT ASSIGNEE(S): SOURCE:

U.S. Pat. Appl. Publ., 103 pp., Cont.-in-part of U.S.

6,406,880. CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

```
PATENT NO.
                 KIND DATE
                                        APPLICATION NO. DATE
     US 2003104513 A1 20030605 US 2002-125647 20020419 <-- WO 9850576 A1 19981112 WO 1998-US8760 19980501 <--
        W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
            DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG,
            KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,
            NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
            UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
            CM, GA, GN, ML, MR, NE, SN, TD, TG
                     B1 20020618
                                        US 1999-429614 19991029 <--
PRIORITY APPLN. INFO.:
                                       US 1997-45512P P 19970502 <--
                                       WO 1998-US8760 A1 19980501 <--
                                       US 1999-429614 A2 19991029
```

#### IT 1462-54-0

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study);

(betaines as adjuvants to susceptibility testing and antimicrobial therapy)

RN 1462-54-0 HCAPLUS

CN β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $Me^-(CH_2)_{11}-NH-CH_2-CH_2-CO_2H$ 

AB The present invention is related to methods and compns. for susceptibility testing of bacteria containing mycolic acid structures using betaine-like detergents, and inducing the susceptibility of such bacteria using the same.

=> d 197 ibib hitstr abs 2-YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

YOU HAVE REQUESTED DATA FROM 7 ANSWERS - CONTINUE? Y/(N):y

L97 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:733825 HCAPLUS

DOCUMENT NUMBER:

131:348769

TITLE:

Compositions and methods for enzymatic decontamination of microbiological samples for analysis and culture

INVENTOR (S): PATENT ASSIGNEE(S):

Thornton, Charles G.; MacLellan, Kerry M. Integrated Research Technology, L.L.C., USA

SOURCE:

U.S., 42 pp.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE US 5985593 A 19991116 US 1997-943338 19971003 <--PRIORITY APPLN. INFO.: US 1996-28470P P 19961011 <--OTHER SOURCE(S): MARPAT 131:348769 1462-54-0, N-Dodecyl- $\beta$ -alanine

RL: BUU (Biological use, unclassified); BIOL (Biological study);

(detergents; compns. and methods for enzymic decontamination of microbiol. samples for anal. and culture)

RN 1462-54-0 HCAPLUS

β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

 $Me^{-(CH_2)_{11}-NH-CH_2-CH_2-CO_2H}$ 

The present invention is related to a method for the enzymic AB decontamination of specimens as a means to control microbiol. contamination. The compns. and methods of the invention are especially useful to eliminate non-gram neg. contaminants of samples being processed for microbiol. anal. Respiratory specimens were processed and treated with N-(3-carboxypropyl)-N,N-dimethyl-1-octadecanaminium, inner salt and with enzyme cocktail containing lysozyme, zymolyase, Trichoderma harzianum extract, and Cytophaga extract

REFERENCE COUNT:

THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L97 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:588589 HCAPLUS

DOCUMENT NUMBER:

119:188589

TITLE: INVENTOR(S): Antiviral composition and method Pollock, Jerry J.; Docherty, John J.

PATENT ASSIGNEE(S):

Northeastern Ohio Universities College of Medicine,

USA

SOURCE:

U.S., 8 pp. Cont.-in-part of U.S. 5,185,153.

CODEN: USXXAM

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT: 2

#### PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5213803	A	19930525	US 1992-840321	19920224 <
US 5185153	A	19930209	US 1990-592552	19901004 <
US 5270032	A	19931214	US 1992-925902	19920806 <
PRIORITY APPLN.	INFO.:		US 1990-592552	19901004 <
			US 1991-671457	19910319 <

7631-98-3 IT

RL: BIOL (Biological study)

(envelope virus-inhibiting pharmaceuticals containing)

7631-98-3 HCAPLUS RN

Glycine, N-dodecyl-N-methyl-, sodium salt (9CI) (CA INDEX NAME) CN

$$\begin{array}{c} & \text{Me} \\ | \\ \text{HO}_2\text{C--} \text{CH}_2\text{--} \text{N--} (\text{CH}_2)_{11}\text{---} \text{Me} \end{array}$$

### Na

A method for killing envelope viruses in vitro causing AIDS and herpes AB infections comprises contacting an infected surface or cavity with an antiviral formulation containing humectant (e.g. sorbitol, glycerol, etc.) 20-80%, and activating agents including inorq. monovalent anions and detergent with carrier or dispenser. The humectant facilitates structural and/or functional 3-dimensional disruption or disorientation of the viral envelope. Various combinations of ingredients in a mouthrinse were tested against herpes simplex virus (HSV)-1. The most potent antiviral activity (>99.9% inhibition) was only seen with all 5 ingredients (sorbitol, Tween 20, NaHCO3, NaSCN, and EtOH) together.

L97 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:512653 HCAPLUS

DOCUMENT NUMBER:

115:112653

TITLE:

Selective modification of the catalytic subunit of

pertussis toxin

INVENTOR(S):

Kaslow, Harvey R.

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S., 10 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DA	ΓE
US 5032398	Α	19910716	US 1986-893080 19	860801 <
US 5165927	Α	19921124	US 1991-682773 19	910409 <
PRIORITY APPLN. II	NFO.:		US 1986-893080 19	860801 <

7631-98-3, Sodium lauryl sarcosine IT

RL: BIOL (Biological study)

(pertussis toxin activation response to, toxin selective alkylation and deactivation in relation to)

RN7631-98-3 HCAPLUS CN Glycine, N-dodecyl-N-methyl-, sodium salt (9CI) (CA INDEX NAME)

$$\begin{array}{c} & \text{Me} \\ | \\ \text{HO}_2\text{C-CH}_2\text{-N-} (\text{CH}_2)_{11}\text{-Me} \end{array}$$

#### Na

AB Pertussis toxin is selectively modified by deactivating key amino acids in the catalytic portion of the toxin, yet leaving the antigenic determinants on the  $\beta$ -oligomer essentially undisturbed. The process involves (1) activating the catalytic subunit with a mixture containing polyphosphate, a sulfhydryl reductant, and a mild detergent; and (2) alkylating the revealed SH groups. Pertussis toxin was incubated with DTT, CHAPS, and ATP for activation and then was alkylated with iodoacetate. The modified toxin gave a 3% NADase activity (untreated was 100%).

L97 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:129164 HCAPLUS

DOCUMENT NUMBER:

114:129164

TITLE:

Surfactant-based dry granular nonalcoholic oral drug

delivery systems

INVENTOR(S):

Wilson, Mark E.; Cole, B. Harrison

PATENT ASSIGNEE(S):

Spectrum Consumer Products Co., Inc., USA U.S., 6 pp. Cont.-in-part of U.S. 4,919,918.

SOURCE:

CODEN: USXXAM

DOCUMENT TYPE:

TYPE: Patent English

LANGUAGE: E. FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4971785	Α	19901120	US 1990-502618	19900330 <
US 4919918	A	19900424	US 1988-167504	19880314 <
CA 1328818	A1	19940426	CA 1989-593151	19890308 <
AU 8931255	A1	19890914	AU 1989-31255	19890313 <
JP 01275521	A2	19891106	JP 1989-63424	19890314 <
JP 2938884	B2	19990825		
CA 2031572	AA	19911001	CA 1990-2031572	19901205 <
CA 2031572	C	19960130		
EP 448895	A1	19911002	EP 1990-403685	19901219 <
EP 448895	B1	19940525		
R: AT, BE,	CH, DE	, ES, FR,	GB, IT, LI, LU, NL	
AT 106012	E	19940615	AT 1990-403685	19901219 <
JP 05017345	A2	19930126	JP 1991-49707	19910314 <
AU 9173693	Al	19910613	AU 1991-73693	19910321 <
AU 635826	B2	19930401		
PRIORITY APPLN. INFO.	:		US 1988-167504	19880314 <
			US 1990-502618	19900330 <
			EP 1990-403685	19901219 <

IT 7631-98-3, Sodium laurylsarcosinate

RL: BIOL (Biological study)

(oral drug formulations containing, granular)

RN 7631-98-3 HCAPLUS

CN Glycine, N-dodecyl-N-methyl-, sodium salt (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ | \\ \text{HO}_2\text{C--} \text{CH}_2\text{--} \text{N--} (\text{CH}_2)_{11}\text{---} \text{Me} \end{array}$$

● Na

AB The compns. comprise surfactants, such as Na laurylsulfate, Na laurylsarcosinate, Na alkylsulfoacetate, etc., spray-dried essential oils, and effervescence-causing components. A composition comprised aspirin 225, surfactant 5, sweetener 95, spray-dried essential oil 400, and effervescence-causing mixture 525 mg. A mouthwash can also be produced by this method.

L97 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1989:552636 HCAPLUS

DOCUMENT NUMBER:

111:152636

 $\mathtt{TITLE}:$ 

Amino acid derivatives as animal growth promoters

Bauwe, Reinhard; Von Rottkay, Fritjof; Schwarz, Justus

PATENT ASSIGNEE(S):

VEB Berlin-Chemie, Ger. Dem. Rep.

SOURCE:

Ger. (East), 3 pp. CODEN: GEXXA8

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

r· 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION	NO.	DATE			
			-						
DD 256073	A1	1988042	.7	DD 1985-282	2385	19851104	<		
RITY APPLN. INFO.	:		DD	1985-282385	5	19851104	<		
R SOURCE(S):	MA	RPAT 111	:152636						
3338-22-5, N-Iso	propyl	glycine	hydrochl	oride.					
RL: AGR (Agricultural use); BIOL (Biological study); USES									
(Uses)									
(feeding expe	riment	with, o	on male r	ats)					
3338-22-5 HCAPL	US								
Glycine, N-(1-me	thylet	hyl)-, h	ydrochlo	ride (9CI)	(CA	INDEX NAME	⊡)		
	DD 256073 RITY APPLN. INFO. R SOURCE(S): 3338-22-5, N-Isc RL: AGR (Agricul (Uses) (feeding expe	DD 256073 A1 RITY APPLN. INFO.: R SOURCE(S): MA 3338-22-5, N-Isopropyl RL: AGR (Agricultural (Uses)     (feeding experiment 3338-22-5 HCAPLUS	DD 256073 A1 1988042 RITY APPLN. INFO.: R SOURCE(S): MARPAT 111 3338-22-5, N-Isopropylglycine RL: AGR (Agricultural use); BI (Uses)     (feeding experiment with, company)	DD 256073 Al 19880427  RITY APPLN. INFO.: DD  R SOURCE(S): MARPAT 111:152636  3338-22-5, N-Isopropylglycine hydrochl RL: AGR (Agricultural use); BIOL (Biol (Uses)	DD 256073 A1 19880427 DD 1985-282385 RITY APPLN. INFO.: DD 1985-282385 R SOURCE(S): MARPAT 111:152636 3338-22-5, N-Isopropylglycine hydrochloride RL: AGR (Agricultural use); BIOL (Biological stud) (Uses) (feeding experiment with, on male rats) 3338-22-5 HCAPLUS	DD 256073 A1 19880427 DD 1985-282385 RITY APPLN. INFO.: DD 1985-282385 R SOURCE(S): MARPAT 111:152636 3338-22-5, N-Isopropylglycine hydrochloride RL: AGR (Agricultural use); BIOL (Biological study); U (Uses) (feeding experiment with, on male rats) 3338-22-5 HCAPLUS	DD 256073 Al 19880427 DD 1985-282385 19851104 RITY APPLN. INFO.: DD 1985-282385 19851104 R SOURCE(S): MARPAT 111:152636 3338-22-5, N-Isopropylglycine hydrochloride RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (feeding experiment with, on male rats)		

i-PrNH-CH2-CO2H

● HCl

GΙ

$$\begin{smallmatrix} H & R^2 & O \\ | & | & | & | \\ R^4 - N - C - C - R^1 \\ | & & \\ R^3 & I \end{smallmatrix}$$

AB Amino acid derivs. I (R1 = OH, NH2, alkoxy, arylamino, alkylamino, dialkylamino; R2, R3 = H, lower alkyl; R4 = C1-5 alkyl) promote growth and feed utilization efficiency when added to animal feed or drinking water, or when applied to the animals mucous membranes. Growing male rats given water ad libitum containing 10 ppm N-isopropylglycine hydrochloride displayed a comparable feed utilization efficiency to those given drinking water containing ambagon/peudothymine.

L97 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1981:71506 HCAPLUS

DOCUMENT NUMBER:

94:71506

TITLE:

Antiseptic composition for topical application to the

skin for use against bromidrosis

INVENTOR(S):

Marcadet, Ernest

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S., 9 pp. Cont. of U.S. Ser. No. 778,358, abandoned.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
US 4224319	A	19800923		US 1979-62409	19790731 <
PRIORITY APPLN.	INFO.:		US	1973-374266	19730627 <
			US	1974-500372	19740826 <
			US	1975-622051	19751114 <
			US	1977-778358	19770317 <

TΤ 76382-07-5

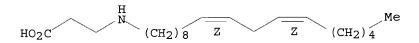
RL: BIOL (Biological study)

(antiseptic composition containing, for bromidrosis treatment)

76382-07-5 HCAPLUS

β-Alanine, N-9,12-octadecadienyl-, (Z,Z)- (9CI) (CA INDEX NAME) CN

Double bond geometry as shown.



An aqueous disinfectant composition, harmless to the skin, contains as the main active agent an amino acid RNH(R1NH)nR2CO2H (R = C8-18 aliphatic; R1 and R2 = C1-3 alkylene; n = 1 or 2), 1 or several triglycerides, and vitamins. Thus, an emulsion was formulated with alkylaminopropionic acid 1.95 g, oleic triglyceride [122-32-7] 6 g, and axerophtol palmitate [79-81-2] 0.6 mg.

L97 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1979:151785 HCAPLUS

DOCUMENT NUMBER:

90:151785

TITLE:

Fungicidal phenylnitramines Cross, Barrington; Dawe, David H.

PATENT ASSIGNEE(S):

American Cyanamid Co., USA

SOURCE:

U.S., 17 pp.

DOCUMENT TYPE:

INVENTOR(S):

CODEN: USXXAM

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4130645	A	19781219	US 1978-879340	19780221 <
DE 2902890	A1	19790823	DE 1979-2902890	19790125 <
AU 7944082	A1	19790830	AU 1979-44082	19790208 <
BR 7900812	Α	19790904	BR 1979-812	19790209 <
EP 3881	A1	19790905	EP 1979-300201	19790209 <
R: CH, FR,	GB, IT	, SE		
DD 143251	C	19800813	DD 1979-211101	19790219 <
DK 7900729	Α	19790822	DK 1979-729	19790220 <
JP 54122233	A2	19790921	JP 1979-19616	19790221 <
PRIORITY APPLN. INFO	. :		US 1978-879340	19780221 <

IT 69733-43-3P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and fungicidal activity of)

RN 69733-43-3 HCAPLUS

CN Butanoic acid, 4-(dodecylamino)-, compd. with 2,3,5,6-tetrachloro-N-nitrobenzenamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 54381-45-2 CMF **C6 H2 C14 N2 O2** 

CM 2

CRN 41421-76-5 CMF **C16 H33 N O2** 

 $Me^-(CH_2)_{11}-NH^-(CH_2)_3-CO_2H$ 

Phenylnitramines RnC6H5-nNR1NO2 (I; R = the same or different halo, Me, CF3, NO2, CN, MeSO2, AcNH, etc.; R1 = H, alkyl, alkenyl, alkynyl, PhCH2, haloalkyl, etc.) and 2,3,5,6-tetrachloro-N-nitroaniline salts 2,3,5,6-Cl4C6HN:N(O)O- M+ (II; M = Na, K, Ba/2, protonated amine, NH4, Me4N, PhCH2NEt3), totalling 99, were prepared I (R1 = H) were prepared by nitration of anilines and were converted to I (R ≠ H) by alkylation, acylation, etc., and II by treatment of 2,3,5,6-Cl4C6HNHNO2 with amines or metal or quaternary ammonium salts. Both I and II showed good fungicidal activity.

### => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:46:44 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 28, 2004 (20040528/UP).

=>

145

06/03/2004

=> fil lreg

FILE 'LREGISTRY' ENTERED AT 08:16:10 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

LREGISTRY IS A STATIC LEARNING FILE

=> fil req

FILE 'REGISTRY' ENTERED AT 08:16:12 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1 DICTIONARY FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:16:29 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil zcaplus

FILE 'ZCAPLUS' ENTERED AT 08:16:33 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

### => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:16:39 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION. R1= unsubstituted LAST RELOADED: May 28, 2004 (20040528/UP). => d que 138 L1 ( 1) SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?) /AU SEL PLU=ON L1 1 RN :  $L_2$ 103 TERMS compounds indexed for application L3 103) SEA FILE=REGISTRY ABB=ON PLU=ON L2 T<sub>1</sub>4 SCR 1518 L5 SCR 2050 2052 2043 SCR 1526 L6 SCR 1235 L7 T.8 CH\sigma CH3 CH√Et H3C√√C√√CH3 @9 10 @11 12 13 @14 15

H3C-\(\sime\) C-\(\sime\) Et 16 @17 18

```
REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
VAR G4=H/CH3
                           no substitutions
NODE ATTRIBUTES:
CONNECT IS E1 RC AT
CONNECT IS E1 RC AT
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18
STEREO ATTRIBUTES: NONE
1.9
                SCR 963
L10 (
        3584468) SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)
                OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)
Ь11 (
            526) SEA FILE=REGISTRY SUB=L10 (SSS FUL) ((L4 AND L6 AND L7 AND L9)
                NOT L5) AND L8
             37) SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT (?NITRILE? OR
L12 (
                ?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS
L13 (
              2) SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND (C6 H13 N O2) /MF AND
                (?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS
L14 (
             39) SEA FILE=REGISTRY ABB=ON PLU=ON L13 OR L12
             16) SEA FILE=REGISTRY ABB=ON PLU=ON (16217-35-9/CRN OR 244189-98-
L15 (
                8/CRN OR 244189-99-9/CRN OR 244190-00-9/CRN OR 244190-01-0/CRN
                OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR
                27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/
                CRN OR 41331-10-6/CRN OR 42313-51-9/CRN)
                                                                 set contains compounds named in application
L16 (
             41) SEA FILE=REGISTRY ABB=ON PLU=ON L14 OR L15
L17
                STR
```

CH3<sub>4</sub>

CH\sqrt CH3 CH√Et H3C√√C√√CH3 @9 10 @11 12

13 @14 15

 $H3C \sim C \sim Et$ 16 @17 18

REP G1 = (1-3) CH2 VAR G2=CH2/9/11/14/17 NODE ATTRIBUTES: CONNECT IS E1 RC AT CONNECT IS E3 RC AT 3 CONNECT IS E1 RC AT DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18 STEREO ATTRIBUTES: NONE

```
L18 STR

2 4 CH^CH3 CH^Et H3C^C^CH3

AK N C C @9 10 @11 12 13 @14 15
```

H3C~~C~~Et 16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E2 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

NUMBER OF N	ODES IS	17		remove quaternary  No (L17 OR L18)  No setts
				remove quality
STEREO ATTR				1) Town HS
L19 (	295)SEA	A FILE=REGISTRY SUB=L3	l1 <i>(</i> SSS FU	(L17 OR L18)
L20 (	976)SEA	A FILE=HCAPLUS ABB=ON	PLU=ON	L19
L21 (	5)SEA	FILE=REGISTRY ABB=O1	1 PLU=ON	I (58482-93-2 OR 42313-51-9 OR
		38-22-5 OR 3183-22-0 (		
		A FILE=REGISTRY ABB=ON		
		A FILE=HCAPLUS ABB=ON		
L24 (	28) SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L23 AND (PY<1999 OR AY<1999
	OR	PRY<1999)		
L25 (	83)SEA	A FILE=HCAPLUS ABB=ON	PLU=ON	L21
L26 (	5)SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L24 AND L25
L27 (	28) SEA	A FILE=HCAPLUS ABB=ON	PLU=ON	L26 OR L24
L28 (	24)SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L20 AND L27
L29	28 SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L27 OR L28
L32	5 SEA	FILE=HCAPLUS ABB=ON	PLU≃ON	(58482-93-2? OR 42313-51-9?)
	(L)	(BIOL OR USES)/RL		,
L33	5 SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L32 AND (PY<1999 OR AY<1999
	OR	PRY<1999)		
L34	14 SEA	FILE=HCAPLUS ABB=ON	PLU=0N	42313-51-9?
L35	14 SEA	FILE=HCAPLUS ABB=ON		L34 AND (PY<1999 OR AY<1999
	OR	PRY<1999)		
L37	1 SEA	FILE=HCAPLUS ABB=ON	PLU=ON	L35 AND (A61K?)/ICM
L38		FILE=HCAPLUS ABB=ON		L37 OR L33 OR L29

=> d 138 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L38 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

```
Reyes 09/646,110
ACCESSION NUMBER:
                          1999:626163 HCAPLUS
DOCUMENT NUMBER:
                          131:243589
TITLE:
                          Aliphatic amino carboxylic and amino phosphonic acids,
                          amino nitriles, and amino tetrazoles as cellular
                          rescue agents
INVENTOR (S):
                          Paterson, I. Alick; Dyck, Lilian E.; Davis, Bruce A.;
                          Liu, Ya-Dong; Durden, David A.; Boulton, Alan A.
PATENT ASSIGNEE(S):
                          University of Saskatchewan Technologies Inc., Can.;
                          The Canada Trust Company
SOURCE:
                          PCT Int. Appl., 52 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:
                          Patent
LANGUAGE:
                          English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                       KIND DATE
                                             APPLICATION NO.
                                                                DATE
                       ----
                             -----
                                             ______
     WO 9948858
                             19990930
                       A2
                                             WO 1999-CA250
                                                                19990325 <--
     WO 9948858
                       A3
                             20000120
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
             DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
             JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
             TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
             MD, RU, TJ, TM
```

```
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
             ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
             CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2325943
                      AA 19990930
                                          CA 1999-2325943 19990325 <--
     AU 9928240
                      A1
                            19991018
                                           AU 1999-28240
                                                            19990325 <--
     AU 767098
                      B2
                            20031030
     TR 200002756
                      Т2
                            20001221
                                           TR 2000-20000275619990325 <--
     EP 1064254
                      A2
                            20010103
                                           EP 1999-908728
                                                          19990325 <--
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
    BR 9909103
                            20011016
                                           BR 1999-9103
                      Α
                                                            19990325 <--
     JP 2002507591
                      Т2
                            20020312
                                           JP 2000-537843
                                                            19990325 <--
     ZA 2000004988
                      Α
                            20010507
                                           ZA 2000-4988
                                                            20000919 <--
    NO 2000004774
                      Α
                            20000925
                                           NO 2000-4774
                                                            20000925 <--
PRIORITY APPLN. INFO.:
                                       US 1998-79488P
                                                         P 19980326 <--
                                       US 1998-79489P
                                                         P 19980326 <--
                                        WO 1999-CA250
                                                         W 19990325
OTHER SOURCE(S):
                        MARPAT 131:243589
    3338-22-5P 31044-48-1P 41331-11-7P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
```

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

RN3338-22-5 HCAPLUS

Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME) CN

 $i-PrNH-CH_2-CO_2H$ ● HCl RN31044-48-1 HCAPLUS CN  $\beta$ -Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME) 0  $MeO-C-CH_2-CH_2-NH-(CH_2)_5-Me$ ● HCl RN41331-11-7 HCAPLUS CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)  $Me^{-(CH_2)_5-NH-CH_2-CH_2-CO_2H}$ IT 3183-21-9P 3183-22-0P 3183-23-1P 16217-35-9P 27453-30-1P 31044-47-0P 40870-77-7P 41331-10-6P 42313-51-9P 56676-69-8P 244189-67-1P 244189-68-2P 244189-69-3P 244189-70-6P 244189-71-7P 244189-72-8P 244189-73-9P 244189-74-0P 244189-75-1P 244189-98-8P 244189-99-9P 244190-00-9P 244190-01-0P 244190-02-1P 244190-03-2P 244190-04-3P 244190-26-9P 244190-27-0P 244190-28-1P 244190-31-6P 244190-32-7P 244190-33-8P 244190-34-9P 244190-37-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

RN 3183-21-9 HCAPLUS

CN Glycine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H

RN 3183-22-0 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{EtO-C-CH}_2\text{-NHPr-i} \end{array}$$

RN 3183-23-1 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

$$\overset{\text{O}}{\parallel}_{\text{EtO-C-CH}_2-\text{NHPr-i}}$$

#### ● HCl

RN 16217-35-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)

$$i-PrNH-CH_2-CH_2-CO_2H$$

RN 27453-30-1 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{tabular}{lll} Me & O \\ & | & | \\ i - Pr - N - CH_2 - CH_2 - C - OMe \\ \end{tabular}$$

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{O} & \\ || & \\ \text{MeO-C-CH}_2\text{--CH}_2\text{--NH--(CH}_2)} & \text{5--Me} \end{array}$$

RN 40870-77-7 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ || \\ \text{MeO-C-CH}_2\text{--CH}_2\text{--NHPr-i} \end{array}$$

# ● HCl

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^-(CH_2)_5-NH-CH_2-CO_2H$ 

RN 42313-51-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

 $Me^-(CH_2)_5-NH-CH_2-CO_2H$ 

# ● HCl

RN 244189-67-1 HCAPLUS CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ● HCl

RN 244189-68-2 HCAPLUS

CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

## ● HCl

RN 244189-69-3 HCAPLUS CN  $\beta$ -Alanine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ● HCl

RN 244189-70-6 HCAPLUS CN  $\beta$ -Alanine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

 $i-PrNH-CH_2-CH_2-CO_2H$ 

# HCl

RN 244189-71-7 HCAPLUS CN Glycine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ● HCl

RN 244189-72-8 HCAPLUS CN Glycine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 244189-73-9 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{tabular}{llll} Me & O & & \\ & & & | & & || \\ i-Pr-N-CH_2-CH_2-C-OMe \\ \end{tabular}$$

● HCl

RN 244189-74-0 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me 
$$(CH_2)_4$$
  $R$  Me  $OMe$ 

● HCl

RN 244189-75-1 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 244189-98-8 HCAPLUS

CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244189-99-9 HCAPLUS

CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} & \text{Me} \\ \text{Me} & \text{HN} \\ \end{array}$$

RN 244190-00-9 HCAPLUS

CN  $\beta$ -Alanine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-01-0 HCAPLUS

CN Glycine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

RN 244190-02-1 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Me$$
 $(CH2)4 S Me$ 
 $HN CO2H$ 

RN 244190-03-2 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-04-3 HCAPLUS

CN β-Alanine, N-methyl-N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-26-9 HCAPLUS

CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-27-0 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)
Absolute stereochemistry.

RN 244190-28-1 HCAPLUS

CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-31-6 HCAPLUS

CN β-Alanine, N-methyl-N-(1-methylethyl) - (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \mid \\ \text{i-Pr-N-CH}_2\text{--CH}_2\text{--CO}_2\text{H} \end{array}$$

RN 244190-32-7 HCAPLUS

CN Glycine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{tabular}{c|c} Me & O \\ & & | & || \\ i-\text{Pr}-N-CH_2-C-OMe \\ \end{tabular}$$

RN 244190-33-8 HCAPLUS

CN Glycine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ || & | \\ \text{MeO-C-CH}_2 - \text{N-(CH}_2) \, \text{5-Me} \end{array}$$

RN 244190-34-9 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

O Me 
$$\parallel$$
  $\parallel$   $\parallel$  MeO-C-CH $_2$ -CH $_2$ -N-(CH $_2$ )5-Me

3/26/25

RN 244190-37-2 HCAPLUS CN  $\beta$ -Alanine, N-hexyl-N-methyl- (9CI) (CA INDEX NAME)

 $\begin{array}{c} & \text{Me} \\ | \\ \text{HO}_2\text{C--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{N--} (\text{CH}_2)_5\text{---}\text{Me} \end{array}$ 

AB Tile compds. R1R2R3CNR4(CH2)nX [R1 = Me(CH2)n (n = 1-16), alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl; R2 = H, Me, Et; R3, R4 = H, Me; X = CO2H or carbalkoxy, cyano, PO3H2 or phosphonate ester, 5-tetrazolyl] or their pharmaceutically acceptable salts were prepared Thus, Me 3-(1-hexylamino)propionate hydrochloride was prepared by addition reaction of 1-hexylamine with Me acrylate and shown to have antiapoptotic activity at 10-6 M.

=> d 138 ibib hitstr abs 2-YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

L38 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1998:675926 HCAPLUS

DOCUMENT NUMBER:

130:3527

TITLE:

Selective addition of amines to methyl acrylate in

presence of alumina

AUTHOR(S):

Suzuki, Yoshitada; Murakami, Shunsuke; Kodomari,

Mitsuo

CORPORATE SOURCE:

Department of Industrial Chemistry, Faculty of

Engineering, Shibaura Institute of Technology,

Minato-ku, Tokyo, 108-8548, Japan

Nippon Kagaku Kaishi (1998), (10), 664-669

CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER:

SOURCE:

Nippon Kagakkai

DOCUMENT TYPE:

Journal Japanese

LANGUAGE:

T 31044-47-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(selective addition of amines to Me acrylate in presence of alumina)

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

 $\begin{tabular}{l} \begin{tabular}{l} \begin{tab$ 

The Michael type addition of primary amines to Me acrylate in benzene was accelerated by alumina, and monoadducts were selectively obtained in high yield. The reaction in benzene did not proceed without alumina. The yields of adducts were dependent on the structure of amines; the monoadducts were obtained in high yield (77-91% yield) when linear amines were used, and in the case of branched or bulky primary amines and secondary amines, the yields were decreased compared to the linear ones. In the addition of diamines to Me acrylate, only an amino group on 1 side of the diamines added to Me acrylate to give the monoadducts selectively, and

the amino group on the another side did not react. In the addition of asym. diamine, the less hindered amino group predominantly reacted with Me acrylate.

L38 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1998:45464 HCAPLUS

DOCUMENT NUMBER:

128:128268

TITLE:

 $_{\ell}$  Solid Phase Synthesis of  $\beta$ -Peptoids:

AUTHOR(S):

N-Substituted β-Aminopropionic Acid Oligomers Hamper, Bruce C.; Kolodziej, Stephen A.; Scates,

Angela M.; Smith, Ronald G.; Cortez, Enriqueta Monsanto Company, St. Louis, MO, 63167, USA

CORPORATE SOURCE: SOURCE:

Journal of Organic Chemistry (1998), 63(3),

708-718

CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society

DOCUMENT TYPE:

PUBLISHER:

Journal

LANGUAGE: English

1462-54-0DP, N-Dodecyl-β-alanine, ester with Wang resin 16217-35-9DP, ester with Wang resin 98430-14-9DP, ester with Wang resin 202059-85-6DP, ester with Wang resin

202059-91-4DP, ester with Wang resin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(solid-phase synthesis of substituted aminopropionic acid oligomers)

RN 1462-54-0 HCAPLUS

CN β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_{11}-NH-CH_2-CH_2-CO_2H}$ 

102 46)

16217-35-9 HCAPLUS RN

β-Alanine, N-(1-methylethyl) - (9CI) (CA INDEX NAME) CN

 $i-PrNH-CH_2-CH_2-CO_2H$ 

RN98430-14-9 HCAPLUS

CNβ-Alanine, N-(2-methylpropyl) - (9CI) (CA INDEX NAME)

i-BuNH-CH2-CH2-CO2H

202059-85-6 HCAPLUS RN

CNβ-Alanine, N-(1-methylpropyl) - (9CI) (CA INDEX NAME)

NH-CH2-CH2-CO2H

Me-CH-Et

202059-91-4 HCAPLUS RN

β-Alanine, N-(2-methylbutyl) - (9CI) (CA INDEX NAME) CN

 $\begin{array}{c} \text{Me} \\ | \\ \text{HO}_2\text{C--} \text{CH}_2\text{---} \text{CH}_2\text{---} \text{NH---} \text{CH}_2\text{---} \text{CH----} \text{Et} \end{array}$ 

IT 202060-00-2P 202060-01-3P 202060-02-4P 202060-06-8P 202060-11-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of substituted aminopropionic acid oligomers)

RN 202060-00-2 HCAPLUS

CN  $\beta$ -Alanine, N-(2-methylpropyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 98430-14-9 CMF C7 H15 N O2

 $\mathtt{i}\,\mathtt{-BuNH}-\mathtt{CH}_2-\mathtt{CH}_2-\mathtt{CO}_2\mathtt{H}$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

F-C-CO<sub>2</sub>H

RN 202060-01-3 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylpropyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 202059-85-6 CMF C7 H15 N O2

 $\begin{array}{c} \mathrm{NH^-\,CH_2^-\,CH_2^-\,CO_2H} \\ | \\ \mathrm{Me^-\,CH^-\,Et} \end{array}$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 202060-02-4 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 16217-35-9 CMF C6 H13 N O2

 $i-PrNH-CH_2-CH_2-CO_2H$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 202060-06-8 HCAPLUS

CN β-Alanine, N-dodecyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 1462-54-0 CMF C15 H31 N O2

 ${\rm Me^-\;(CH_2)_{\,11}^-\,NH^-\,CH_2^-\,CH_2^-\,CO_2H}$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 202060-11-5 HCAPLUS

CN  $\beta$ -Alanine, N-(2-methylbutyl)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 202059-91-4 CMF C8 H17 N O2

 $\begin{array}{c} \text{Me} \\ | \\ \text{HO}_2\text{C--} \text{CH}_2\text{--} \text{CH}_2\text{--} \text{NH--} \text{CH}_2\text{--} \text{CH---} \text{Et} \end{array}$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

GΙ

 $\ensuremath{\mathtt{AB}}$   $\ensuremath{\mathtt{A}}$  solid-phase organic synthesis method has been developed for the preparation of

N-substituted- $\beta$ -aminopropionic acid oligomers or  $\beta$ -peptoids I. Treatment of polymer-bound 4-(benzyloxy)benzyl acrylate with primary amines afforded N-substituted  $\beta$ -alanines. Polymer loadings and

product conversions were determined by direct cleavage of resin-bound materials and measurement by 1H NMR with an internal standard. The NMR method was used to establish loading of all resin-bound intermediates including acrylic acid. Acylation with acryloyl chloride followed by Michael addition of primary amines to the acrylamide allowed preparation of di- $\beta$ -peptoids. By a linear set of seven reactions, trimeric N-benzyl- $\beta$ -aminopropionic acid was prepared in 67% overall yield. Single-bead FT-IR microspectroscopy was used to acquire spectra of the resin bound mono- $\beta$ -peptoids, di- $\beta$ -peptoids, and acrylamide intermediates. A combinatorial library of defined mixts. of tri- $\beta$ -peptoids was prepared by mixing equimolar amts. of the mono- $\beta$ -peptoid resins and carrying them through two sequences of the acylation-Michael addition. The identity of a sample mixture II (R = Me, CH2Ph, CH2CH2Ph, CH2C6H4OMe-4, allyl, CH2CHMe2, CHMeEt, CHMe2) was determined by LC-MS anal. of the cleavage product.

REFERENCE COUNT:

THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1996:637648 HCAPLUS

DOCUMENT NUMBER:

INVENTOR(S):

126:24866

TITLE:

Desensitizing solution for offset printing plate

Itakura, Ryosuke; Kasai, Seishi; Sera, Hidefumi; Kato,

Eiichi

PATENT ASSIGNEE(S):

Fuji Photo Film Co., Ltd., Japan

SOURCE:

U.S., 35 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	K	IND	DATE		APPLICATION NO.	DATE	
. 1								
\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	US 5565290		A	19961015		US 1992-920862	19920728	<
]	US 5723239		A	19980303		US 1996-718949	19960926	<
PRIC	ORITY APPLN.	INFO.:			JP	1991-190081	19910730	<
					JP	1991-269609	19911017	<
					JP	1991-269917	19911018	<
					JP	1991-269918	19911018	<
					JP	1991-320488	19911204	<
					US	1992-920862	19920728	<

OTHER SOURCE(S):

MARPAT 126:24866

IT 1462-54-0 41331-11-7 101816-76-6

RL: TEM (Technical or engineered material use); USES (Uses) (offset printing plate preparation by electrophotog. using desensitizing solns. containing phytic acid derivative and)

RN 1462-54-0 HCAPLUS

CN β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $Me^- (CH_2)_{11} - NH^- CH_2 - CH_2 - CO_2H$ 

RN 41331-11-7 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_5-NH-CH_2-CH_2-CO_2H}$ 

```
101816-76-6 HCAPLUS
RN
```

β-Alanine, N-(2-ethylhexyl) - (9CI) (CA INDEX NAME) CN

```
CH2-NH-CH2-CH2-CO2H
Et-CH-Bu-n
```

AΒ An amine compound-containing, but cyanogen-free, desensitizing solution for an offset printing plate prepared from an electrophotog. material, characterized by containing phytic acid and/or a metal and/or ammonium salts of phytic acid and at least one imide compound containing 1-6 amino groups of formula -NR1R2 and 1-6 imide bonds of the formula -CON(R3)CO- (R1, R2 = H or an organic group or R1 and R2 together may form a cyclic structure; R3 = H, halogen, cyano, nitro, or an organic group).

L38 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:878827 HCAPLUS

DOCUMENT NUMBER:

123:286739

TITLE:

Preparation of N-alkylated amino acid and peptide

chelating agents and their chelates with

radionuclides.

INVENTOR(S):

Spies, Hartmut; Schulze, Paul-Eberhard; Noll, Bernd;

Noll, Steffi; Dinkelborg, Ludger

PATENT ASSIGNEE(S):

Institut fuer Diagnostikforschung GmbH an der Freien

Universitaet Berlin, Germany

SOURCE:

Ger. Offen., 32 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

				DATE		APPLICATION NO.	DATE	
						DE 1993-4337600		
ZA	9408411		Α	19950630		ZA 1994-8411	19941026 <	
WO	9512610		A1	19950511		WO 1994-DE1295	19941027 <	
	W: AU,	CA,	CN, HU	, JP, KR,	NO,	US		
	RW: AT,	BE,	CH, DE	, DK, ES,	FR,	GB, GR, IE, IT, LU	, MC, NL, PT,	SE
CA	2173844		AA	19950511		CA 1994-2173844	19941027 <	
AU	9481038		A1	19950523		AU 1994-81038	19941027 <	
				19970911				
EP	726909		A1	19960821		EP 1995-900059	19941027 <	
	R: AT,	BE,	CH, DE	, DK, ES,	FR,	GB, GR, IE, IT, LI	, LU, MC, NL,	PT, SE
CN	1134158		Α	19961023		CN 1994-193990	19941027 <	
HU	74881		A2	19970228		HU 1996-1140	19941027 <	
							19941027 <	
NO	9601743		A	19960430		NO 1996-1743	19960430 <	
PRIORITY	Y APPLN.	INFO.	:		D	E 1993-4337600	19931101 <	
					W	O 1994-DE1295	19941027 <	
OTHER SO	OURCE(S):		MAI	RPAT 123:	28673	39		

IT 41331-10-6P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-alkylated amino acid and peptide chelating agents and their chelates with radionuclides)

RN41331-10-6 HCAPLUS

CNGlycine, N-hexyl- (9CI) (CA INDEX NAME)  $Me^- (CH_2)_5 - NH^- CH_2 - CO_2H$ 

R3SCH2CONR1(CH2CONH)nCH2COR2 [n = 0-2; R1 = (0-interrupted or O-substituted) alkyl, carboxyalkyl, hydroxyalkyl, aminoalkyl, etc., (substituted) Ph, cyclohexyl, etc.; R2 = halo, halomethyl, MeCO, NH2, OH, etc.; R3 = H, Ac, PhCO, acetamidomethyl, EtS, trityl, etc.], were prepared Thus, glycine anhydride in aqueous NaOH was treated with ClCH2COCl at 0° to give ClCH2CO-Gly-Gly-OH, which was kept with hexylamine in EtOH to give Me(CH2)5-Gly-Gly-Gly-OH. The latter was stirred with ClCH2COCl in aqueous NaOH and the product was stirred with thiobenzoic acid in MeOH to give N-(benzoylmercaptoacetyl)-N-hexylglycylglycylglycine, which was hydrogenolyzed to give N-(mercaptoacetyl)-N-hexylglycylglycylglycine, the 99mTc complex of which was used to image atherosclerotic changes in rabbits.

L38 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:777639 HCAPLUS

DOCUMENT NUMBER:

123:198616

TITLE:

Preparation of N-sulfonylindoline derivatives with affinity for vasopressin and oxytocin receptors Wagnon, Jean; de Cointet, Paul; Nisato, Dino;

INVENTOR(S):

Plouzane, Claude; Sereadeil-Legal, Claudine; Tonnerre,

Bernard

PATENT ASSIGNEE(S):

Elf Sanofi SA, Fr.

SOURCE:

U.S., 50 pp. Cont.-in-part of U.S. Ser. No.737,655,

abandoned. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5338755	Α	19940816	US 1992-923839	19920803 <
FR 2665441	A1	19920207	FR 1990-9778	19900731 <
FR 2665441	B1	19921204		
IL 114934	A1	19960804	IL 1991-114934	19910730 <
HU 219351	В	20010328	HU 1971-99045	19910731 <
FR 2679903	A1	19930205	FR 1991-9908	19910802 <
FR 2679903	B1	19931203		
AU 9224758	A1	19930302	AU 1992-24758	19920731 <
AU 658664	B2	19950427		
BR 9205336	A	19931116	BR 1992-5336	19920731 <
JP 06501960	T2	19940303	JP 1993-503337	19920731 <
RU 2104268	C1	19980210	RU 1993-5168	19920731 <
IL 117592	A1	19990411	IL 1992-117592	19920731 <
CZ 288173	В6	20010516	CZ 1993-682	19920731 <
CA 2206776	C	20020226	CA 1992-2206776	19920731 <
SK 283463	B6	20030805	SK 1993-426	19920731 <
NO 9301262	A	19930526	NO 1993-1262	19930401 <
NO 180047	В	19961028		
NO 180047	C	19970205		
US 5397801	А	19950314	US 1994-240360	19940510 <
US 5481005	A	19960102	US 1994-348150	19941128 <
US 5578633	A	19961126	US 1995-458614	19950602 <
FI 9800175	Α	19980127	FI 1998-175	19980127 <

PRIORITY APPLN. INFO.:

```
FR 1990-9778
                A 19900731 <--
US 1991-737655
                B2 19910730 <--
FR 1991-9908
                A 19910802 <--
IL 1991-99012
                A3 19910730 <--
HU 1991-2552
                A 19910731 <--
CA 1992-2093221 A3 19920731 <--
CS 1993-682
                A 19920731 <--
IL 1992-102703
               A3 19920731 <--
WO 1992-FR758
                A 19920731 <--
US 1992-923839
               A3 19920803 <--
FI 1993-1476
                A 19930401 <--
US 1993-923839
                A3 19930803 <--
US 1994-240360
                A3 19940510 <--
US 1994-348150
               A3 19941128 <--
```

OTHER SOURCE(S):

MARPAT 123:198616

IT 42313-51-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-sulfonylindoline derivs. with affinity for vasopressin and oxytocin receptors)

RN 42313-51-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

GΙ

Title compds. I (R'1 = halo, C1-4 alkyl, HO, C1-4 alkoxy, PhCH2O, NC, F3C, O2N, H2N; R'2 = C1-6 alkyl, C3-7 cycloalkyl, C5-7 cycloalkylene, (substituted) Ph, etc.; R'3 = H; R'4 = H2NCO, R'6R'7NCO wherein R'6R'7N = saturated 5-membered substituted N-heterocyclyl; R'5 = C1-4 alkyl, 1-, 2-naphthyl, (substituted) Ph, etc.; n = m = 0-2) or a salt thereof, are prepared CH2BrCONMe2 (preparation given) and 5-chloro-2-(tosylamino)phenyl cyclohexyl ketone were reacted to give 2-[N-tosyl-N-(dimethylcarbamoylmethyl)amino]-5-(chlorophenyl) cyclohexyl ketone which in THF was treated with Li diisopropylamide to give after workup trans-I (R'1n = 5-Cl, R'2 = cyclohexyl, R'3 = H, R'4 = Me2NCO, R'5 = 4-MeC6H4, m = 0). The IC50 of I affinity for oxytocin receptors was 10-5-10-8M.

L38 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1993:46312 HCAPLUS

DOCUMENT NUMBER:

118:46312

TITLE:

Solubilization of copper(II) complexes of N-alkyl- $\beta$ -alanines in their micellar solutions

```
AUTHOR(S):
                           Nakamura, Akio; Koshinuma, Masakatsu; Tajima, Kazuo
CORPORATE SOURCE:
                           Nagoya Munic. Women's Coll., Nagoya, 464, Japan
SOURCE:
                           Colloids and Surfaces (1992), 67, 183-93
                           CODEN: COSUD3; ISSN: 0166-6622
DOCUMENT TYPE:
                           Journal
                           English
LANGUAGE:
     27373-56-4, N-Decyl-β-alanine 27373-57-5
     41331-11-7 77390-89-7, N-Butyl-\beta-alanine
     RL: PRP (Properties)
         (micelles, copper(II) complex solubilization in)
     27373-56-4 HCAPLUS
RN
     β-Alanine, N-decyl- (8CI, 9CI) (CA INDEX NAME)
Me^{-(CH_2)_9} - NH^{-CH_2} - CH_2 - CO_2H
     27373-57-5 HCAPLUS
     β-Alanine, N-octyl- (6CI, 8CI, 9CI) (CA INDEX NAME)
Me^-(CH_2)_7 - NH^-CH_2 - CH_2 - CO_2H
RN
     41331-11-7 HCAPLUS
CN
     β-Alanine, N-hexyl- (9CI)
                                 (CA INDEX NAME)
Me^{-(CH_2)}_{5}-NH^{-CH_2}-CH_2-CO_2H
     77390-89-7 HCAPLUS
RN
     β-Alanine, N-butyl- (9CI)
                                 (CA INDEX NAME)
n-BuNH-CH_2-CH_2-CO_2H
IT
     27373-56-4D, N-Decyl-\beta-alanine, copper(II) complexes
     27373-57-5D, copper(II) complexes 41331-11-7D,
     copper(II) complexes 77390-89-7D, N-Butyl-\beta-alanine,
     copper(II) complexes
     RL: PROC (Process)
         (solubilization of, in alkyl-\beta-alanine micellar solns.)
RN
     27373-56-4 HCAPLUS
     β-Alanine, N-decyl- (8CI, 9CI) (CA INDEX NAME)
CN
Me^{-(CH_2)_9} - NH^{-CH_2} - CH_2 - CO_2H
RN
     27373-57-5 HCAPLUS
CN
     β-Alanine, N-octyl- (6CI, 8CI, 9CI) (CA INDEX NAME)
Me^- (CH_2)_7 - NH^- CH_2 - CH_2 - CO_2H
RN
     41331-11-7 HCAPLUS
CN
     β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)
```

```
Me^- (CH_2)_5 - NH^- CH_2 - CH_2 - CO_2H
```

77390-89-7 HCAPLUS RΝ

 $\beta$ -Alanine, N-butyl- (9CI) (CA INDEX NAME) CN

 $_{\mathrm{n-BuNH}-\,\mathrm{CH}_2-\,\mathrm{CH}_2-\,\mathrm{CO}_2\mathrm{H}}$ 

The solubilization of the Cu(II) N-alkyl- $\beta$ -alanine complexes (NAA; AB alkyl = Bu, NBuA; hexyl, NHeA; octyl, NOA; decyl, NDeA)) in NAA aqueous micellar solns. was studied. A crystalline coordination compound of Cu:NAA composition 1:2 (the complex trans-[Cu(NAA)2(H2O)2]) is formed by direct mixing of NAA with CuCl2 aqueous solns. The amount of the insol. stoichiometric 1:2 complex increases with increasing NAA concentration below the NAA critical

micelle concentration (CMC), but the 1:2 complex begins to redissolve above the CMC and disappears at a certain NAA concentration (i.e., the insol. 1:2 complex is solubilized in the NAA micelles). Visible spectroscopic data suggest that the dielec. environment around the Cu(II) ion coordination sphere in the solubilized 1:2 complex is similar to that in the crystalline 1:2 complex mol. Lamellar structures of NAA micelles solubilizing the 1:2 complexes were characterized by small-angle x-ray diffractometry. A model for the solubilization is proposed: 2 hydrocarbon chains in a 1:2 complex mol. of trans form are interlinked with the NAA bilayers. The free energy of solubilization was estimated from the solubilized amts. of the 1:2 complexes for the NDeA and NOA systems. The change in the free energy of solubilization per CH2 group is -1.04 kJ mol-1, which is roughly half of the corresponding value for soap micellization.

```
L38 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
```

ACCESSION NUMBER:

1992:59021 HCAPLUS

DOCUMENT NUMBER:

116:59021

TITLE:

Diethyl bromophosphate as a new condensing reagent for

the formation of  $\beta$ -lactams from  $\beta$ -amino

acids

AUTHOR(S):

Chung, Bong Young; Paik, Kyu Cheol; Nah, Cha Soo Dep. Chem., Korea Univ., Seoul, 136-701, S. Korea

Bulletin of the Korean Chemical Society (1991

CORPORATE SOURCE: SOURCE:

), 12(5), 589

CODEN: BKCSDE; ISSN: 0253-2964

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 116:59021

16217-35-9

RL: RCT (Reactant); RACT (Reactant or reagent) (lactamization of, by bromophosphate)

16217-35-9 HCAPLUS RN

 $\beta$ -Alanine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

 $i-PrNH-CH_2-CH_2-CO_2H$ 

GΙ

AB  $\beta$ -Lactams I (R = CH2Ph, CHMe2, H; R1, R3 = H, Me; R2 = H, Me, CO2Me, Ph) were obtained in 25-89% yield by cyclizing HO2CCHR1CR2R3NHR with BrP(O)(OEt)2.

L38 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:631922 HCAPLUS

DOCUMENT NUMBER:

115:231922

TITLE:

A convenient method for the  $\beta$ -lactam formation from  $\beta$ -amino acids using triphenylphosphine-

hexachloroethane-triethylamine-acetonitrile system Chung, Bong Young; Paik, Kyu Cheol; Nah, Cha Soo Dep. Chem., Korea Univ., Seoul, 136-701, S. Korea

CORPORATE SOURCE:

AUTHOR(S):

Bulletin of the Korean Chemical Society (1991

SOURCE:

Bulletin of the Korean Chemical Society (199: ), 12(4), 456

DOCUMENT TYPE:

CODEN: BKCSDE; ISSN: 0253-2964

LANGUAGE:

Journal English

IT 16217-35-9

RL: RCT (Reactant); RACT (Reactant or reagent) (intramol. cyclocondensation of,  $\beta$ -lactam from)

RN 16217-35-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)

i-PrNH-CH2-CH2-CO2H

GΙ

AB Intramol cyclocondensation of RNHCR1R2CHR3CO2H (R = H, CHMe2, CH2Ph; R1 = H, Me, Ph, CO2Me; R2, R3 = H, Me) in the presence of the title reagent/solvent system gave 70-92%  $\beta$ -lactams I.

L38 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:27105 HCAPLUS

DOCUMENT NUMBER:

114:27105

TITLE:

Absorbent composition containing a severely-hindered amine mixture with amine salts and/or amino acid additives for the absorption of hydrogen sulfide

INVENTOR(S):

Ho, W. S. Winston; Sartori, Guido; Stogryn, Eugene L. Exxon Research and Engineering Co., USA

PATENT ASSIGNEE(S):

SOURCE:

U.S., 19 pp. Cont. of U.S. Ser. No. 106,782,

abandoned. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 4961873 A 19901009 US 1989-398346 19890824 <-PITTY APPIN. INFO.: US 1987-106782 19871013 <--

PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 114:27105

58482-93-2, N-tert-Butylglycine

RL: USES (Uses)

(absorbents containing, two severely-hindered amines in, for selective removal of hydrogen sulfide from gases)

58482-93-2 HCAPLUS RN

Glycine, N-(1,1-dimethylethyl) - (9CI) (CA INDEX NAME)

t-BuNH-CH2-CO2H

AΒ An alkaline absorbent solution that reduces the H2S content in a treated gas to <10 ppm contains 2 severely-hindered amines, e.g., bis(tbutylaminoethoxy) ethane and ethoxyethoxyethanol-tert-butylamine, a severely-hindered amine salt, and/or a severely-hindered amino acid. The process is also suitable for the selective removal of H2S from liquid mixts. comprising H2S and CO2.

L38 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:201962 HCAPLUS

DOCUMENT NUMBER:

112:201962

TITLE:

Addition of severely-hindered amine salts and/or amino

acids to non-hindered amine solutions for the

absorption of hydrogen sulfide

INVENTOR(S):

Ho, W. S. Winston; Sartori, Guido

PATENT ASSIGNEE(S):

Exxon Research and Engineering Co., USA

SOURCE:

U.S., 13 pp.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 4892674 A 19900109 US 1987-106805 19871013 <-RITY APPLN. INFO: US 1987-106805 19871013 <--

PRIORITY APPLN. INFO.: US
OTHER SOURCE(S): MARPAT 112:201962

IT 58482-93-2, N-tert-Butylglycine

RL: USES (Uses)

(absorbents containing, and severely-hindered amine salts and non-hindered amines, for hydrogen sulfide removal from gases)

RN 58482-93-2 HCAPLUS

Glycine, N-(1,1-dimethylethyl) - (9CI) (CA INDEX NAME)

t-BuNH-CH2-CO2H

Page 27

An alkaline absorbent solution for the selective removal of H2S from a H2S-containing

gas contains the additive of a severely-hindered amine salt, e.g., ethoxyethanol-tert-butylamine, and/or a severely-hindered amino acid,

e.g., N-tert-butylalanine, to a non-hindered amine such as

N-methyldiethaolamine (I). The H2S-removal process is also suitable for the gas mixts. containing H2S and CO2. Use of the above absorbent solution leads

to higher selectivity for H2S than observed when I is used alone.

L38 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1990:182789 HCAPLUS

DOCUMENT NUMBER:

112:182789

TITLE:

Addition of severely hindered amino acids to severely hindered amines for absorption of hydrogen sulfide

INVENTOR(S):

Sartori, Guido; Ho, W. S. Winston

PATENT ASSIGNEE(S):

Exxon Research and Engineering Co., USA

SOURCE:

U.S., 10 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_\_\_ US 1987-106795 19871013 <--US 4895670 A 19900123 US 1987-106795 19871013 <-PTTY APPLN. INFO.: US 1987-106795 19871013 <--PRIORITY APPLN. INFO.:

OTHER SOURCE(S): CASREACT 112:182789

58482-93-2, N-tert-Butylglycine ΤT

RL: USES (Uses)

(absorbents containing severely hindered amines and, for absorption of hydrogen sulfide)

58482-93-2 HCAPLUS RN

Glycine, N-(1,1-dimethylethyl) - (9CI) (CA INDEX NAME) CN

t-BuNH-CH2-CO2H

A process for the removal of H2S from fluid mixts. comprises using an alkaline ABabsorbent solution containing a severely hindered amino acid and a severely hindered amine each having a cumulative -Es value (Taft's steric hindrance constant) >1.75. The process is also suitable for the selective removal of H2S from fluid mixts. containing H2S and CO2. Use of the absorbent solution leads to higher selectivity for H2S than observed when the severely hindered amine is used alone without the severely hindered amino acid. Suitable amino acid includes N-tert-butylalanine, N-tert-butylqlycine, and their mixture

L38 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1989:38631 HCAPLUS

DOCUMENT NUMBER:

110:38631

TITLE:

Preparation and use of acylaminopropionates as surfactants, emulsifiers, wetteners, detergent components, and in production of waterproof leather Dahmen, Kurt; Mertens, Richard; Stockhausen, Dolf

INVENTOR(S):

Chemische Fabrik Stockhausen G.m.b.H., Fed. Rep. Ger.

PATENT ASSIGNEE(S): SOURCE:

Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

	TENT NO.			DATE	APPLICATION NO. DATE	
DE	3717961 3717961		A1	19880505 19940526	DE 1987-3717961 19870527 <-	
EP	265818 265818		A2 A3		EP 1987-115365 19871021 <-	-
	265818	מם	B1	19940928	GB, GR, IT, LI, NL, SE	
	6311254	4	A2	19880517	JP 1987-266178 19871021 <-	· –
ES	2577011 2003836		Т3	19970129 19941216		
	8780101 602171		A1 B2	19880428 19901004	AU 1987-80101 19871023 <-	-
	8705693 1833368		A A3	19880531 19930807	BR 1987-5693 19871023 <- SU 1989-4613176 19890104 <-	
	2062302 11044		C1 B	19960620 19961020	RU 1989-4613251 19890104 <- LV 1993-715 19930628 <-	
LT	3617 3805		B B	19951227 19960325	LT 1993-1535 19931206 <-	
	Y APPLN.	INFO.	_	19900325	DE 1986-3636497 19861027 <-	-
					DE 1987-3717961 19870527 <-	-

OTHER SOURCE(S):

MARPAT 110:38631

IT 112-87-8P 10488-59-2P 41331-11-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acylation of, by maleic anhydride)

RN 112-87-8 HCAPLUS

CN β-Alanine, N-octadecyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_{17}-NH-CH_2-CH_2-CO_2H}$ 

RN 10488-59-2 HCAPLUS

CN  $\beta$ -Alanine, N-(9Z)-9-octadecenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

$$_{\text{HO}_2\text{C}}$$
 $_{\text{N}}$ 
 $_{\text{(CH}_2)}$ 
 $_{\text{8}}$ 
 $_{\text{Z}}$ 
 $_{\text{(CH}_2)}$ 
 $_{\text{7}}$ 
 $_{\text{Me}}$ 

RN 41331-11-7 HCAPLUS

CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^- (CH_2)_5 - NH^- CH_2 - CH_2 - CO_2H$ 

AB R1(R2A)NCH2CHR3CO2X [R1 = C1-22 (unsatd.) alkyl, alkoxyalkyl; R2 = C1-18 alkyl, C3-4 carboxyalkyl, carboxyphenyl, carboxy; R3 = H, Me; X = H, alkali metal, alkaline earth metal, (alkyl)ammonium alkanolammonium; A = C0, SO2, CONH, C0-3 alkylene] useful as emulsifiers, wetteners, surfactants,

and in preparation of waterproofing agents for leather, were prepared by reaction

of R1NH2 with (meth)acrylic acid followed by acylation with carboxylic acid anhydrides, carbonyl chlorides, isocyanates, etc. Thus, CH2:CHCO2H was added to oleylamine at 60° and after 2.5 h and 90° maleic anhydride was added and the mixture was stirred for a further 2 h at 70-80° to give N-oleyl-N-(2-carboxyethyl) maleamic acid. The latter was used to prepare waterproof leather.

L38 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1987:440328 HCAPLUS

DOCUMENT NUMBER:

107:40328

TITLE:

Amine dealkylation

INVENTOR (S):

Miller, William Harold; Balthazor, Terry Mack

PATENT ASSIGNEE(S):

Monsanto Co., USA

SOURCE:

Eur. Pat. Appl., 14 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 199702	A1	19861029	EP 1986-870047	19860421 <
EP 199702	В1	19881221		
R: AT, BE, C	H, DE	, FR, GB, IT,	, LI, LU, NL, SE	
US 4804500	A	19890214	US 1986-841149	19860319 <
DK 8601811	A	19861023	DK 1986-1811	19860421 <
AU 8656410	A1	19861030	AU 1986-56410	19860421 <
AU 580153	B2	19890105		
JP 61249955	A2	19861107	JP 1986-91967	19860421 <
JP 06062522	B4	19940817		
ZA 8602986	Α	19870225	ZA 1986-2986	19860421 <
HU 43998	A2	19880128	HU 1986-1665	19860421 <
HU 199399	В	19900228		
AT 39349	E	19890115	AT 1986-870047	19860421 <
CA 1269665	A1	19900529	CA 1986-507122	19860421 <
IL 78551	A1	19901223	IL 1986-78551	19860421 <
PRIORITY APPLN. INFO.:			US 1985-725856	19850422 <
			EP 1986-870047	19860421 <

#### 3183-21-9 108957-96-6 IT

RL: RCT (Reactant); RACT (Reactant or reagent) (N-deisopropylation of)

3183-21-9 HCAPLUS RN

Glycine, N-(1-methylethyl) - (9CI) (CA INDEX NAME) CN

 $i-PrNH-CH_2-CO_2H$ 

108957-96-6 HCAPLUS RN

Glycine, N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME) CN

Мe i-Pr-N-CH2-CO2H

Substituted amines R1NR2R3 [R1 = acidic group containing at least one OH; R2 = H, Me, PhCH2, R1, R3; R3 = CR4R5CHR6R7; R2R3N = heterocyclyl; R4, R5 = H, C1-6 alkyl, (un) substituted aryl; R6, R7 = R4, R5, OH, C1-6 alkoxy, aryloxy, halo, SH, thioalkyl, mono- or dialkylamino, or, when R6 = H, R7 can be N(CH2CO2H)2] were dealkylated by heating at 250-400° in aqueous alkali, using at least the stoichiometric amount of alkali needed to neutralize the acidic OH groups, to give R1R2NH with removal of R3 groups as alkenes. The process is useful for preparation of valuable amino acids, e.g., glycine, sarcosine, iminodiacetic acid, and aminomethylphosphonic acid. Thus, a solution of 0.038 mol Me2CHNMeCH2CO2H in H2O containing 0.076 mol

NaOH was heated at 300° in an Monel autoclave to give 71% sarcosine.

L38 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1986:462332 HCAPLUS

DOCUMENT NUMBER:

105:62332

TITLE:

Surface treatment of zinc base materials

INVENTOR(S):

Kurihara, Masao; Kimata, Shizuro; Imura, Hideaki;

Naruse, Naohiko

PATENT ASSIGNEE(S):

Toa Gosei Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Tokkyo Koho, 9 pp.

CODEN: JAXXAD

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

]	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
			<b></b>		
Ċ	JP 60056225	B4	19851209	JP 1978-102938	19780825 <
į	JP 55031417	<b>A</b> 2	19800305		
R.	ITY APPLN. INFO.	:		JP 1978-102938	19780825 <

PRIORITY APPLN. INFO.: 41331-11-7 41421-76-5

RL: USES (Uses)

(pretreatment by aqueous alkalies and, of zinc, for coating with powdered epoxy resin)

41331-11-7 HCAPLUS RN

CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^-(CH_2)_5-NH-CH_2-CH_2-CO_2H$ 

RN 41421-76-5 HCAPLUS

CN Butanoic acid, 4-(dodecylamino) - (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_{11}-NH^{-(CH_2)_3-CO_2H}}$ 

AΒ Surfaces of zinc are treated with aqueous alkali hydroxide and aqueous solns. of

RNHCnH2nCO2H (R = >C6 saturated or unsatd. aliphatic hydrocarbyl groups, n > 2) or H halide solns. and coated. Thus, Zn-plated steel was degreased, treated with 6% aqueous KOH, immersed 5 min at 90° in 3% aqueous hexyl- $\beta$ -aminopropionic acid, dried, electrostatically coated with a powdered epoxy resin, and baked to form a coating.

L38 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:73067 HCAPLUS DOCUMENT NUMBER: 104:73067 TITLE: Effect of surfactants on the formation of a metallic film during metalizing of glass fibers AUTHOR(S): Ermakov, E. A.; Pantaev, V. A. CORPORATE SOURCE: Kalinin. Gos. Univ., Kalinin, USSR Khim. Poverkhn.-Akt. Veshchestv Kompleksonov ( SOURCE: **1984**), 107-10. Editor(s): Gorelov, I. P. Kalinin. Gos. Univ.: Kalinin, USSR. CODEN: 54JOAA DOCUMENT TYPE: Conference LANGUAGE: Russian 41331-11-7 IT RL: USES (Uses) (surfactant, in electroless copper coating of glass fibers, film d. and structure in relation to) 41331-11-7 HCAPLUS RNβ-Alanine, N-hexyl- (9CI) (CA INDEX NAME) CN $Me^-(CH_2)_5-NH-CH_2-CH_2-CO_2H$ AΒ The effect of surfactants, i.e. Na alkylsulfates and alkyl- $\beta$ -alanine on the formation of a metal film during electroless Cu coating of glass fibers was studied. Elec. resistance of the fibers metalized without surfactants was substantially higher than that of samples prepared using the surfactants, which was associated with the difference in the Cu film surface defectiveness. Coatings obtained using the surfactants were distinguished by the fine-crystalline structure, whereas without them, coarser crystallites formed, and the coating was less dense. The best results in preparing dense coatings with fine-grained structure were observed when electroless bath contained Na undecylsulfate [1072-24-8] and N-hexyl-β-alanine [ 41331-11-7]. L38 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1986:24719 HCAPLUS DOCUMENT NUMBER: 104:24719 TITLE: Effect of inorganic salts of tin and palladium on colloidal-chemical properties of surfactants Voronchikhina, L. I.; Pavlova, L. A. AUTHOR(S): CORPORATE SOURCE: Kalinin. Gos. Univ., Kalinin, USSR SOURCE: Khim. Poverkhn.-Akt. Veshchestv Kompleksonov ( 1984), 88-92. Editor(s): Gorelov, I. P. Kalinin. Gos. Univ.: Kalinin, USSR. CODEN: 54JOAA DOCUMENT TYPE: Conference LANGUAGE: Russian 41331-11-7 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

 $Me^- (CH_2)_5 - NH^- CH_2 - CH_2 - CO_2H$ 

41331-11-7 HCAPLUS

RN

CN

The behavior of colloidal solns. of surfactants (amphoteric AB

β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

(surface activity of, in presence of tin or palladium chlorides)

N-dodecyl-N, N-dimethyl- $\alpha$ -betain and N-ketyl- $\beta$ -alanine; anionic Na cetyl sulfate and Na undecyl sulfate and cationic decylpyridinium chloride and dodecylbenzyldimethylammonium chloride) was studied in the presence of SnCl2 and PdCl2. The saturated adlayer formation, critical micellization concentration, and surface tension were determined At < 0.5M SnCl2 and

PdCl2 in solns., surface activity of the amphoteric and anionic surfactants increases significantly. The cationic surfactants are unstable in the presence of > 0.05M surfactants.

L38 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1980:147180 HCAPLUS

DOCUMENT NUMBER:

92:147180

TITLE:

Cation-binding cyclic peptides with lipophilic tails

AUTHOR(S):

Deber, C. M.; Adawadkar, P. D.

CORPORATE SOURCE:

Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8,

SOURCE:

Biopolymers (1979), 18(10), 2375-96

CODEN: BIPMAA; ISSN: 0006-3525

DOCUMENT TYPE:

Journal

LANGUAGE:

English

20933-56-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and esterification of, with benzyl alc.)

20933-56-6 HCAPLUS

Glycine, N-decyl- (8CI, 9CI) (CA INDEX NAME)

 $Me^{-}(CH_2)_9 - NH^{-}CH_2 - CO_2H$ 

41331-10-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

41331-10-6 HCAPLUS

Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-}$  (CH<sub>2</sub>)<sub>5</sub>-NH-CH<sub>2</sub>-CO<sub>2</sub>H

Cyclo[Glu(OCH2Ph)-Sar-Gly-NRCH2CO]2 (I; Sar = NMeCH2CO, R = Me) was prepared AB by coupling BOC-Glu(OCH2Ph)-Sar-Gly-Sar-OH (BOC = Me3CO2C) to H-Glu(OCH2Ph)-Sar-Gly-Sar-OH by the mixed anhydride method, esterifying the resulting octapeptide with HOC6H4NO2-p, BOC-deblocking the resulting p-nitrophenyl ester with HCl, and cyclizing the resulting H-[Glu(OCH2Ph)-Sar-Gly-Sar]2-OC6H4NO2-p in DMF/pyridine at high dilution I [R = decyl (II), hexyl, cyclohexyl], cyclo[Glu(OCH2Ph)-Sar-Gly-Sar-Glu(OCH2PH)-Sar-Gly-NR1CH2CO]2 (R1 = decyl), and cyclo(Phe-Sar-Gly-Sar)2 were also prepared, and the above  $\alpha\text{-benzyl}$  esters were converted to the free acids. Proton and 13C NMR data showed that I with a mixture of cis/trans peptide bond conformers were converted to the C2-sym. all-trans conformers upon complexation with Ca2+. II mediated the transport of cations across a thick-liquid membrane with the following selectivity: Ca2+ > Na+ > K+ > Mn2+ > Cu2+ > Mg2+ > Co2+ > Zn2+.

L38 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1977:135270 HCAPLUS

DOCUMENT NUMBER:

86:135270

TITLE:

Facilitated diffusion of amino acids across

bimolecular lipid membranes as a model for selective accumulation of amino acids in a primordial protocell

AUTHOR(S): Stillwell, William

CORPORATE SOURCE:

Dep. Biophys., Michigan State Univ., East Lansing, MI,

USA

SOURCE:

BioSystems (1976), 8(3), 111-17 CODEN: BSYMBO; ISSN: 0303-2647

DOCUMENT TYPE:

Journal English

LANGUAGE:

627-01-0 3182-81-8 41331-10-6

50997-13-2

RL: PEP (Physical, engineering or chemical process); PROC (Process) (diffusion of, across lipid membrane)

RN 627-01-0 HCAPLUS

CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $\mathtt{EtNH}-\mathtt{CH}_2-\mathtt{CO}_2\mathtt{H}$ 

RN 3182-81-8 HCAPLUS

CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 ${\tt n-BuNH-CH_2-CO_2H}$ 

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}_{5} - NH^{-CH_2} - CO_2H$ 

RN 50997-13-2 HCAPLUS

CN Glycine, N-nonyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)} 8^{-NH-CH_2-CO_2H}$ 

As simple transport system for the uptake of amino acids into lipid vesicles was studied as a model for the protocell. The rate of diffusion of amino acids across bimol. lipid membranes was greatly stimulated by water-soluble aldehydes. Even HCHO was an effective carrier, although pyridoxal was much more effective. Series of reduced amino acid imines of glycine, lysine, and histidine were synthesized to measure the relative abilities of different aldehydes as carriers for amino acids. Comparison of partition coeffs. to the diffusion rates of the derivatized amino acids indicated that the more lipophilic derivs. are more readily diffused. This simple type of facilitated diffusion makes lipid vesicles an attractive model of the 1st primoridal cell.

L38 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1976:430029 HCAPLUS

DOCUMENT NUMBER:

85:30029

TITLE:

Oxidation of sarcosine and N-alkyl derivatives of

glycine by D-amino-acid oxidase

AUTHOR(S):

Naoi, Makoto; Yagi, Kunio

CORPORATE SOURCE: SOURCE:

Fac. Med., Univ. Nagoya, Nagoya, Japan Biochimica et Biophysica Acta (1976),

438(1), 61-70

CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE:

Journal English

LANGUAGE:

IT

627-01-0 3182-81-8 25303-14-4

35386-27-7 41331-10-6

RL: BIOL (Biological study)

(amino acid oxidase specificity for)

RN 627-01-0 HCAPLUS

CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH2-CO2H

RN 3182-81-8 HCAPLUS

CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH2-CO2H

RN 25303-14-4 HCAPLUS

CN Glycine, N-propyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

 $n-PrNH-CH_2-CO_2H$ 

RN 35386-27-7 HCAPLUS

CN Glycine, N-pentyl- (6CI, 9CI) (CA INDEX NAME)

 $Me^- (CH_2)_4 - NH^- CH_2 - CO_2H$ 

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}_{5}-NH^{-CH_2}-CO_2H$ 

AB Sarcosine was oxidized by D-amino acid oxidase (EC 1.4.3.3) to yield methylamine and glyoxylic acid. A series of N-alkyl glycines were also oxidized by this enzyme. N-acetyl- and N-phenylglycine inhibited the oxidase by competing with the substrate, whereas N-methyl-N-acetylglycine did not bind to the enzyme. This suggests the requirement of at least 1 unsubstituted H atom at the amino group of glycine for binding. The primary step in the reaction was the release of a proton from the substrate, indicating the formation of a substituted imino acid, which was spontaneously hydrolyzed to glyoxylic acid and an amine.

L38 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1975:514857 HCAPLUS

DOCUMENT NUMBER:

83:114857

TITLE:

Preparation of N-alkyl and N-arylglycines from glyoxylic acid using carbonylhydridoferrate as a

reducing agent

AUTHOR(S):

Watanabe, Yoshihisa; Shim, Sang Chul; Mitsudo, Takeaki; Yamashita, Masakazu; Takegami, Yoshinobu

CORPORATE SOURCE: SOURCE:

Fac. Eng., Kyoto Univ., Kyoto, Japan Chemistry Letters (1975), (7), 699-700

CODEN: CMLTAG; ISSN: 0366-7022

Journal

DOCUMENT TYPE:

English

LANGUAGE:

3182-82-9P 56676-69-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

3182-82-9 HCAPLUS RN

Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

n-BuNH-CH2-CO2H

● HCl

56676-69-8 HCAPLUS RN

Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}_{5} - NH^{-CH_2} - CO_2H$ 

#### ● HCl

To Fe(CO)5 and alc. in KOH was added an amine, glyoxylic acid and EtOH and the mixture stirred 24 hr at room temperature The precipitate was acidified with concentrate

HCl to give salts of glycines, RNHCH2CO2H·HCl (R = Me, Bu, hexyl, cyclohexyl, PhCH2, Ph, p-MeC6H4, p-MeOC6H4, p-ClC6H4, β-naphthyl.

L38 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1975:409540 HCAPLUS

DOCUMENT NUMBER:

83:9540

TITLE:

Alkyl 5-oxoalkanoates

INVENTOR(S):

Mueller, Werner Farbwerke Hoechst A.-G.

PATENT ASSIGNEE(S): SOURCE:

Ger. Offen., 11 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

FAMILY ACC. NUM. COUNT:

German

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DATE
DE 2325160	A1	19741205	DE 1973-2325160 19730518 <
ZA 7402951	Α	19750528	ZA 1974-2951 19740508 <
IN 141915	Α	19770430	IN 1974-CA1033 19740509 <
NL 7406400	Α	19741120	NL 1974-6400 19740513 <
CH 593902	Α	19771230	CH 1974-6689 19740515 <
IT 1012464	A	19770310	IT 1974-22850 19740516 <

```
FR 2229679
                            19741213
                       A1
                                          FR 1974-17272
                                                           19740517 <--
                       Bl
     FR 2229679
                            19781117
                       A2
     JP 50030829
                            19750327
                                           JP 1974-54612
                                                           19740517 <--
     BE 815282
                       A1
                            19741120
                                          BE 1974-144528 19740520 <--
     GB 1473184
                       Α
                            19770511
                                          GB 1974-22412 19740520 <--
PRIORITY APPLN. INFO.:
                                        DE 1973-2325160
                                                            19730518 <--
     42313-51-9
     RL: CAT (Catalyst use); USES (Uses)
         (catalyst, for ketone addition to alkyl acrylates)
     42313-51-9 HCAPLUS
RN
     \beta\text{-Alanine, N-(1-methylethyl)-, methyl ester (9CI)} (CA INDEX NAME)
CN
MeO-C-CH2-CH2-NHPr-i
     Fifteen RCOCHR1CH2CHR2CO2R3 [R = Me, Et, Bu, or Ph; R1 = H, Me, Pr, or Ph;
     or RR1 = (CH2)4; R2 = H or Me; R3 = C1-4 alkyl] or their mixts. were
     prepared by reaction of RCOCH2R1 with CH2:CR2CO2R3 in the presence of
     amines. Thus, Me2CO and CH2:CHCO2Me were autoclaved in the presence of
     aqueous Me2CHNH2 and BzOH at 180° to give 84.5% MeCO(CH2)3CO2Me and <
     10% (MeO2CCH2CH2) 2CHCOMe.
L38 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        1974:888 HCAPLUS
DOCUMENT NUMBER:
                         80:888
TITLE:
                        Diffusion of glycine and N-substituted glycines across
                        bimolecular lipid membranes
AUTHOR(S):
                         Stillwell, William; Winter, Harry C.
CORPORATE SOURCE:
                        Dep. Biochem., Pennsylvania State Univ., University
                         Park, PA, USA
SOURCE:
                         Biochemical and Biophysical Research Communications (
                         1973), 54(4), 1437-43
                         CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                        English
     627-01-0 3182-81-8 41331-10-6
     50997-13-2
     RL: PEP (Physical, engineering or chemical process); PROC (Process)
        (diffusion of, across liposome)
RN
     627-01-0 HCAPLUS
     Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
EtNH-CH2-CO2H
RN
     3182-81-8 HCAPLUS
     Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
n-BuNH-CH_2-CO_2H
RN
    41331-10-6 HCAPLUS
CN
    Glycine, N-hexyl- (9CI) (CA INDEX NAME)
```

```
Me^-(CH_2)_5-NH-CH_2-CO_2H
```

RN50997-13-2 HCAPLUS Glycine, N-nonyl- (9CI) (CA INDEX NAME) CN

 $Me^{-(CH_2)}8^{-NH}CH_2-CO_2H$ 

Free glycine diffused very slowly across synthetic bimol. lipid membranes, AB whereas several N-substituted derivs. of glycine penetrated the membranes more readily. Pyridoxal, formaldehyde, and acetaldehyde enhanced the diffusion of glycine across the membranes, presumably the result of imine formation between the aldehyde and the  $\alpha$ -amino group of glycine. Several N-substituted glycines were synthesized and their rates of efflux from liposomes were related to their H2O-CHCl3 partition coeffs. This is the 1st demonstration of carrier-mediated diffusion of amino acids across a bimol. lipid membrane.

L38 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1973:101277 HCAPLUS

DOCUMENT NUMBER:

78:101277

TITLE:

Synergistic combinations for inhibiting the attack of

alkaline solutions on alkali-sensitive substrates

Dupre, Jean; Booman, Keith A.

INVENTOR(S): PATENT ASSIGNEE(S):

Rohm and Haas Co.

SOURCE:

U.S., 7 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3653095	A	19720404	US 1969-835906	19690618 <
GB 1320793	A	19730620	GB 1970-29430	19700617 <
PRIORITY APPLN.	INFO.:		US 1969-834499	19690618 <
			US 1969-835906	19690618 <

1462-54-0 41331-10-6 41331-11-7 IT

RL: USES (Uses)

(corrosion inhibition by, of alkaline solns.)

RN 1462-54-0 HCAPLUS

β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

```
Me^{-(CH_2)_{11}-NH-CH_2-CH_2-CO_2H}
```

41331-10-6 HCAPLUS RN

Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_5-NH^-CH_2-CO_2H}$ 

41331-11-7 HCAPLUS RN

β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}_{5} - NH^{-CH_2} - CH_2 - CO_2H$ 

During cleaning with an aqueous alkaline solution containing 0.1-10 weight % AΒ alkali,

materials (e.g. Al, Zn, Sn, Pb, their alloys, Si oxides and compds. containing Si oxides) which are sensitive to the alkaline attack are protected by a synergistic combination of: ≥1 metal ion (0.005M) such as Ba2+, Ca2+, and Sr2+ with ≥1 surface-active agent (0.5 weight %) selected from alkyl glycosides having a formula ROGmH, where G is a glycosyl radical, R is C6-16 alkyl connected to C-1 of the glycosyl radical through the 0, and m = 1-4; or ethylene oxide adducts of the alkyl glycosides containing ≤2 ethylene oxide units per glycosyl radical; or amino carboxylic acids having C≥10 and metal salts of amino carboxylic acids (0.01-5 weight %). Optionally in certain and essentially in other applications, a H2O-soluble naphthalene derivative may be added to the synergistic combination.

L38 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1973:38037 HCAPLUS

DOCUMENT NUMBER:

78:38037

TITLE:

Potential hypotensive compounds. Substituted

3-aminopropionates and 3-aminopropionohydroxamic acids Biggs, D. F.; Coutts, R. T.; Selley, M. L.; Towill, G.

AUTHOR (S):

CORPORATE SOURCE:

Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB,

SOURCE:

Journal of Pharmaceutical Sciences (1972),

61(11), 1739-45

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE:

LANGUAGE:

Journal English

TΤ

40870-77-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and hypotensive effect of)

40870-77-7 HCAPLUS RN

β-Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA CNINDEX NAME)

0 MeO-C-CH2-CH2-NHPr-i

● HCl

Most of the 48 3-aminoproprionate esters studied were synthesized by addition AΒ of an amine across the  $\alpha,\beta\text{-double}$  bond of Me acrylate [96-33-3], Me methacrylate [80-62-6], or Me crotonate [18707-60-3], while the remainder were obtained by interaction of 1 mole of a 3-bromopropionic ester with 2 moles of the corresponding amine. Twenty-six 3-aminopropionohydroxamic acid hydrochlorides were prepared by treatment of the appropriate amino ester with hydroxylamine-HCl [5470-11-1] in MeOH. Many of the compds. such as 2-methyl-3-[(2-phenylethyl)amino]propanoic acid Me ester [6297-67-2], 3,3'-[(2-phenylethyl)imino]bispropanoic acid dimethyl ester [38129-46-3], N-[3-(hydroxyamino)-2-methyl-3oxopropyl]heptanaminium chloride [38129-47-4], and N-[3-(hydroxyamino)-3-oxopropyl]-2-(2-phenylethyl)benzeneethanaminium chloride [38202-84-5] possessed hypotensive properties but of very short duration. 2-Methyl-3-(octylamino)propanoic acid Me ester [29228-46-4] was the most active, and at 4 mg/kg i.v. decreased the blood pressure of rats by an average of 52% for 12 min. Some of the compds. were screened for their ability to protect mice against a lethal dose of diisopropylfluorophosphate [55-91-4], but none was active.

L38 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1971:75986 HCAPLUS

DOCUMENT NUMBER:

74:75986

TITLE:

Synthesis and properties of some hypotensive

N-alkylaminopropionic esters and N,N-

dialkylaminopropionic esters and their hydroxamic

acids

AUTHOR(S):

Coutts, Ronald T.; Hubbard, J. W.; Midha, Kamal K.;

Prasad, Kailash

CORPORATE SOURCE:

Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB,

Can.

SOURCE:

Journal of Pharmaceutical Sciences (1971),

60(1), 28-33

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE:

Journal English

LANGUAGE:

10478-41-8P 31044-47-0P 31044-48-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 10478-41-8 HCAPLUS

CN  $\beta$ -Alanine, N-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

 $EtNH-CH_2-CH_2-CO_2H$ 

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

 $\begin{array}{c|c} & & & & \\ & & & & \\ \text{MeO}-\text{C}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{(CH}_2)}_5-\text{Me} \end{array}$ 

RN 31044-48-1 HCAPLUS

CN β-Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)

 $\begin{tabular}{ll} & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$ 

● HCl

GI For diagram(s), see printed CA Issue.

AB Thirty-eight 3-(N-alkylamino) - and 3-(N,N-dialkylamino) propionic esters

(I), hydroxamic acids (II), carboxylic acids, and related compds. were synthesized and the majority of the esters and hydroxamic acids decreased the blood pressure of anesthetized cats, while the carboxylic acids were inactive. The esters were prepared by the interaction of methyl acrylate or methyl methacrylate and an appropriate amine. Some hindered amines did not react with the acrylate, and some esters hydrolyzed to the corresponding carboxylic acids when stored even for a short time. hydroxamic acids were prepared from the amino esters treated with hydroxylamine.

L38 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1970:445265 HCAPLUS

DOCUMENT NUMBER:

73:45265

TITLE:

Derivatives of substituted acetic acids. XXVIII.

Dialkylaminopropyl esters of  $\alpha$ naphthylheterylacetic acids

AUTHOR (S):

Mndzhovan, A. L.; Badalyan, V. E. Inst. Tonkoi Org. Khim., Erevan, USSR

CORPORATE SOURCE: SOURCE:

Armyanskii Khimicheskii Zhurnal (1970),

23(4), 258-67

CODEN: AYKZAN; ISSN: 0515-9628

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

27453-30-1P TT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

27453-30-1 HCAPLUS RN

β-Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX CN NAME)

A mixture of 0.5 mole R1R2NH, 0.5 mole CH2: CHCO2Me, in 200 ml C6H6 refluxed ABfor 6-8 hr (with iso-PrR2NH, the mixture was heated at 95° in a sealed tube 16-20 hr while with (iso-Pr)2NH similarly treated for 150 hr, to give R1R2NCH2CH2CO2Me (I). LiAlH4 reduction of (I) gave R1R2NCH2CH2CH2OH (II) which, in refluxing PhMe, reacted with  $\alpha\text{-CloH7CHClCOCl}$  (III) [from  $\alpha$ -C10H7CH(OH)CO2H (50.5 g) and refluxing SOCl2 (180 ml)] to give the corresponding  $\alpha\textsc{-C10H7CHClCO2}\,\textsc{(CH2)}\,\textsc{3NR1R2}$  (IV). IV treated with an amine yielded the title  $\alpha\text{-C10H7CHR3CO2}\left(\text{CH2}\right)3\text{NR1R2}$  (V). Thus a mixture of 0.025 mole IV, 0.05 mole piperidine, and 100 ml PhMe refluxed 6-8 hr gave 77% V (R1 = R2 = Me, R3 = piperidino), b3  $228-30^{\circ}$ . The morpholino analog was similarly prepared Approx. 150 new compds. and derivs. were reported.

L38 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1967:517255 HCAPLUS

DOCUMENT NUMBER:

67:117255

TITLE:

Preparation of N-substituted aspartic esters,  $\beta\text{-amino}$  esters, and their corresponding acids

Pfau, Michel AUTHOR(S):

CORPORATE SOURCE:

Lab. Chim. Ecole Norm. Super., Paris, Fr. Bulletin de la Societe Chimique de France (

SOURCE:

**1967**), (4), 1117-25

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE:

Journal

```
LANGUAGE:
                         French
OTHER SOURCE(S):
                         CASREACT 67:117255
     16217-35-9P 16270-07-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and N.M.R. of)
RN
     16217-35-9 HCAPLUS
CN
     β-Alanine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)
i-PrNH-CH2-CH2-CO2H
RN
     16270-07-8 HCAPLUS
CN
     β-Alanine, N-propyl- (8CI, 9CI) (CA INDEX NAME)
n-PrNH-CH_2-CH_2-CO_2H
     Et acrylate (I), diethyl fumarate (II), dimethyl maleate (III),
AB
     MeCH: CHCO2Et (IV), and CH2: CMeCO2Me (V) are treated with PrNH2, iso-PrNH2,
     and Et2NH to give amino acids. Thus, a mixture of 0.05 mole I and 0.5 mole
     PrNH2 is kept 24 hrs. to give Et \beta-propylaminopropionate, b0.1
     32°. A mixture of 5.0 g. I and 1.5 g. PrNH2 is refluxed 10 hrs. to
     give diethyl \beta,\beta'-propyliminodipropionate, b0.4 98°.
     Also prepared are (reactants, product, b.p./mm., and m.p. given): iso-PrNH2
     and I, iso-PrNHCH2CH2CO2Et, 38°/0.4, -; iso-PrNH2 and I,
     iso-PrN(CH2CH2CO2Et)2, 92°/0.05, -; Et2NH and I, Et2NCH2CH2CO2Et,
     28°/0.08, -; PrNH2 and IV, MeCH(NHPr)CH2CO2Et, 36°/0.15, -;
     iso-PrNH2 and IV, Me(iso-PrNH)CHCH2CO2Et, 77°/11, -; PrNH2 and V,
     PrNHCH2CHMeCO2Me, 31°/0.15, -; iso-PrNH2 and V,
     iso-PrNHCH2CHMeCO2Me, 41°/0.1, -; PrNH2 and III,
     MeO2CCH2CH(NHPr)CO2Me, 65-6°/0.15, -; iso-PrNH2 and III,
     MeO2CCH2CH(NHPr-iso)CO2Me, 70°/0.3, -; Et2NH and III,
     MeO2CCH(NEt2)CH2CO2Me, 64°/0.3, -; PrNH2 and II,
     EtO2CCH(NHPr)CH2CO2Et, 91°/0.3, -; iso-PrNH2 and II,
     EtO2CCH(NHPr-iso)CH2CO2Et, 84°/0.4, -; Et2NH and II,
     EtO2CCH(NEt2)CH2CO2Et, 62°/0.1, -; piperidine and III, di-Me
     N, N-pentamethyleneaspartate, 98-101°/0.5, 44-4.5°;
     piperidine and III, Me \alpha-piperidino-\beta-
     piperidinocarbonylpropionate, -, 182-3° (decomposition). Also prepared
     are iso-PrNHCHMeCH2CO2Et-HCl, m. 118.5-19.5°, and iso -
     PrNHCH2CHMeCO2Me.HCl, m. 114-14.5°. The esters are hydrolyzed to
     qive the following acids (m.p. given): PrNHCH2CH2CO2H, 150.5-1.5°;
     iso-PrNHCH2CH2CO2H, 165-6°; Et2NCH2CH2CO2H, 68-70°;
     Me(PrNH)CHCH2CO2H, 142-3°; Me(iso-PrNH)CHCH2CO2H, 165-6°;
     PrNHCH2CHMeCO2H, 136-7°; iso-PrNHCH2CHMeCO2H, 170.5-1.0°;
     MeO2C(PrNH)CHCH2CO2H, 151°; MeO2C(iso-PrNH)CHCH2CO2H,
     120.5-21°; EtO2C(PrNH)CHCH2CO2H, 165-7°;
     EtO2C (iso-PrNH) CHCH2CO2H, 94-5°, HO2CCH (NHPr-iso) CH2CO2H,
     170-2°. N.M.R. data are given for the prepared compds.
L38 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         1966:451518 HCAPLUS
DOCUMENT NUMBER:
                         65:51518
ORIGINAL REFERENCE NO.: 65:9660q-h,9661a
                         Systemic fungicides
TITLE:
INVENTOR(S):
                         Harnack, Willy: Schwarz, Justus
SOURCE:
                         3 pp.
DOCUMENT TYPE:
                         Patent
```

LANGUAGE:

Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DD 45884 19660205 DD 19641224 <-GB 1048507 GB

RN 542-53-0 HCAPLUS

CN Glycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

 $\mathtt{EtNH}-\mathtt{CH}_2-\mathtt{CO}_2\mathtt{H}$ 

● HCl

RN 627-01-0 HCAPLUS CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH2-CO2H

RN 3182-82-9 HCAPLUS CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

 $n-BuNH-CH_2-CO_2H$ 

● HCl

RN 3182-86-3 HCAPLUS CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-BuNH-CH2-CO2H

● HCl

RN 3183-23-1 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME) Eto-C-CH2-NHPr-i

● HCl

3338-22-5 HCAPLUS RNGlycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME) CN

i-PrNH-CH2-CO2H

● HCl

6939-13-5 HCAPLUS RNGlycine, N-propyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

 $n-PrNH-CH_2-CO_2H$ 

### ● HCl

Glycine derivs. of the general formula RHNCH2CO2R' (R = H, Me, or Et) were AB systemic fungicides in vivo but not in vitro (spore germination test). Four young tomato plants with 4 or 5 leaves, in plastic pots were treated 2 times at 2-day intervals at the root stock with 3 ml. of test solution Two days later they were sprayed with a spore suspension of Phytophthora infestans, then placed in a moist chamber. After 4 days each plant was scored for fungus infestation on scale 0, 1, 2, 3, or 4 meaning no, mild, median, marked infestation, or plant destroyed, resp. Scores for water alone and for each fungicide in replicate rests were summed. The sum for water was set at 100, and the relative scores of fungicides recorded. For 8 plants so treated with N-ethylglycine (I), N-ethylglycine-HCl (II), N-propylglycine-HCl (III), and N-2-hydroxyethylglycine (IV) in 0.5% solns., the relative infection scores were 0, 6, 10, 11, resp., and for 0.25% solns. 12, 10, 25, 20, resp. Eight plants sprayed sop. with solns. of II, III, and N-isopropylglycine-HCl were protected to a similar extent. Celery plants were protected against Septoria apii by root stock immersion in 0.5 and 0.25% solns. of the methyl esters and the methyl ester hydrochlorides of N-isopropylglycine and N-allylglycine, the Et ester of N-allylglycine, and N-butylglycine, N-isobutylglycine hydrochlorides. Areas of infection were usually smaller than in the controls. Development of reproductive structures is practically completely depressed.

L38 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1965:480952 HCAPLUS

DOCUMENT NUMBER:

63:80952

ORIGINAL REFERENCE NO.: 63:14970h,14971a-b

TITLE:

Monoalkylated glycine derivatives

AUTHOR (S):

Hanke, H.

CORPORATE SOURCE:

Univ. Jena, GA

SOURCE:

Pharmazeutische Zentralhalle fuer Deutschland ( 1960), 99 (June), 318-22

From: CZ 1963(26), 10820-1. CODEN: PHZEAD; ISSN: 0369-9773

DOCUMENT TYPE:

Journal

German LANGUAGE:

542-53-0, Glycine, N-ethyl-, hydrochloride 627-01-0, IT Glycine, N-ethyl- 3182-81-8, Glycine, N-butyl- 3182-82-9 , Glycine, N-butyl-, hydrochloride 3182-85-2, Glycine, N-isobutyl- 3182-86-3, Glycine, N-isobutyl-, hydrochloride 3182-89-6, Glycine, N-isohexyl- 3182-90-9, Glycine, N-isohexyl-, hydrochloride 3183-21-9, Glycine, N-isopropyl-3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1, Glycine, N-isopropyl-, ethyl ester, hydrochloride 3338-22-5,

Glycine, N-isopropyl-, hydrochloride

(preparation of) 542-53-0 HCAPLUS

RNGlycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

EtNH-CH2-CO2H

● HCl

RN627-01-0 HCAPLUS Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH2-CO2H

3182-81-8 HCAPLUS RNGlycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH2-CO2H

3182-82-9 HCAPLUS RNGlycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

 $n-BuNH-CH_2-CO_2H$ 

HCl

3182-85-2 HCAPLUS RNGlycine, N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

i-BuNH-CH2-CO2H

3182-86-3 HCAPLUS RN

CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

 $i-BuNH-CH_2-CO_2H$ 

### ● HCl

RN 3182-89-6 HCAPLUS CN Glycine, N-isohexyl- (7CI, 8CI) (CA INDEX NAME)

 $Me_2CH-(CH_2)_3-NH-CH_2-CO_2H$ 

RN 3182-90-9 HCAPLUS CN Glycine, N-isohexyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

 $Me_2CH-(CH_2)_3-NH-CH_2-CO_2H$ 

## HCl

RN 3183-21-9 HCAPLUS CN Glycine, N-(1-methylethyl)- (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H

RN 3183-22-0 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

 $\overset{\text{O}}{\parallel}_{\text{EtO-C-CH}_2-\text{NHPr-i}}$ 

RN 3183-23-1 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

 $\begin{array}{c} \text{O} \\ \parallel \\ \text{EtO-C-CH}_2\text{--NHPr-i} \end{array}$ 

### ● HCl

RN 3338-22-5 HCAPLUS CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)  $i-PrNH-CH_2-CO_2H$ 

● HCl

Primary amine HCl salts with HCHO and KCN yield alkylamino-acetonitriles AB which can be hydrolyzed with alc. HCl to N-alkylglycines Et ester HCl salts. These treated with NH3-CHCl3 yield the free esters which are converted by acid saponification to the alkylglycine (Ia) and their HCl salts. Thus, to obtain N-ethylglycine (I), m. 180-2° (decomposition), I.HCl is treated with AgOH in water, the mixture filtered, the filtrate gassed with H2S, filtered, concentrated, and the residue dissolved in EtOH-Et2O. I.HCl m. 179-80°, is prepared by boiling 3 hrs. the Et ester (II) in 6N HCl, evaporating, and dissolving in EtOH-Et20. To prepare II.HCl, m. 135°, HCHO, EtNH2.HCl, and KCN are allowed to react 30 min. in aqueous solution at 5° under CO2, the mixture kept several hrs., the nitrile formed extracted with Et20 (yield 90-100%), boiled 4 hrs. with ethanolic HCl, the NH4Cl filtered off and the filtrate concentrated; yield 90-100%. II, b16 58°, is obtained by 30-min. reaction of II.HCl and NH3-CHCl3 at 0° filtering and distilling; yield 55-75%. Similarly were prepared the following Ia (alkyl, m.p., m.p. HCl salt, b.p. Et ester, and m.p. Et ester HCl salt given): isopropyl, 193-5° (decomposition), 202-3°, b2-3 32-5°, 113-15° (decomposition); allyl, 158-9° (decomposition), 167-9° (decomposition), b3 47°, 113-14° (decomposition) (EtOH); n-butyl,  $190\overline{-1}^{\circ}$  (decomposition),  $202\overline{-4}^{\circ}$ ,  $b2\overline{-3}$  47-51°, 164-6°; isobutyl, 192-3° (decomposition), 210-12° (decomposition) or 221-222° (in sealed tube), b3 49-51°, 127-8.5° (decomposition); isohexyl, 194-5°, 186-7° b4 79°, 182-3°.

L38 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

1963:435 HCAPLUS ACCESSION NUMBER:

58:435 DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 58:63e

Physicochemical analysis of isopropylamine-ethyl TITLE:

monochloroacetate system

Bekturov, E. A. AUTHOR(S):

Izvestiya Akademii Nauk Kazakhskoi SSR, Seriya SOURCE:

Khimicheskaya (1962), (1), 44-8

CODEN: IKAKAK; ISSN: 0002-3205

Journal DOCUMENT TYPE: Russian

LANGUAGE: 3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1,

Glycine, N-isopropyl-, ethyl ester, hydrochloride

(formation of)

3183-22-0 HCAPLUS RN

Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C-CH2-NHPr-i

RN 3183-23-1 HCAPLUS Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

Eto- C- CH2-NHPr-i

#### ● HCl

Measurement of viscosity, d., and conductivity of system Me2CHNH2 + CH2-ClCO2Et AΒ shows the formation of (Me2CHNH2CH2CO2Et)+.-Cl-, which then reacts with the 2nd mol. of amine to form Me2CHNHCH2CO2Et and Me2CHNH3Cl.

L38 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1956:52502 HCAPLUS

DOCUMENT NUMBER:

50:52502

ORIGINAL REFERENCE NO.: 50:10024h-i,10025a-d

TITLE:

The preparation of substituted hydrazines. III. A general method for preparing N-substituted glycines

AUTHOR(S):

Tien, Jack M.; Hunsberger, I. Moyer Antioch Coll., Yellow Springs, O.

CORPORATE SOURCE:

SOURCE:

Journal of the American Chemical Society (1955

), 77, 6696-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

TT

Journal

LANGUAGE:

Unavailable 56676-69-8, Glycine, N-hexyl-, hydrochloride

(preparation of)

56676-69-8 HCAPLUS RN

Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME) CN

 $Me^{-(CH_2)_5-NH-CH_2-CO_2H}$ 

#### ● HCl

cf. C.A. 50, 3431c. C6H13NH2 (0.765 g.) and 1.7 g. HOCH2CO2Et (62% pure) in 10 cc. glacial AcOH allowed to stand 2 hrs., hydrogenated with shaking 2 hrs. at room temperature and 3-4 atmospheric pressure over 0.1 g. 10% Pd-C,

colorless filtrate neutralized with solid NaHCO3 and extracted with two 60-cc. portions Et20, the residue from the extract refluxed 10 min. with 5 cc. 10% aqueous NaOH, cooled, and acidified with 2-3 cc. concentrated HCl, and the

precipitated

small, nearly white plates, m. 200-6°, heated with 25 cc. glacial AcOH on a steam bath, filtered hot, and cooled gave 0.4 g. N-hexylglycine (I) HCl salt, white flakes, m. 215-18°. The filtrate from the hydrogenation basified with dilute aqueous NaOH, refluxed cooled, acidified

with

excess concentrated HCl, and evaporated to dryness, and the residue extracted with hot

glacial AcOH gave I.HCl. C6H13NH2 and HOCH2CO2Et in 2:3 concentrated HCl-H2O gave only a very low yield of I.HCl; no I.HCl was detected from a hydrogenation in 6N HCl. PhNH2 (1.00 g.) in 5 cc. 95% EtOH and 1.70 g.

HOCH2CO2Et (62% pure) hydrogenated 2.5 hrs. and filtered, the catalyst washed with 10 cc. 95% EtOH, and the combined filtrate and washings diluted to the cloud point with H2O and cooled gave 1.06 g. N-phenylglycine Et ester (II), white plates, m. 57-8°; 2nd and 3rd crops, 0.41 and 0.17 g., resp. II (0.179 g.) refluxed 10 min. with 2 cc. concentrated HCl and

cc. H2O and evaporated to dryness in vacuo, the white residue dissolved with warming with 2 cc. concentrated HCl on the steam bath, and the solution cooled gave

0.116 g. N-phenylglycine-HCl salt, m. 172-4°; 2nd crop, 0.041 g. Com. N-phenylglycine (0.1 g.), yellow powder, and 0.1 g. NaCl dissolved at about 70° in 5 cc. H2O, and the solution cooled deposited after about 2 min. large pale-yellow needles; a similar recrystn. in the presence of 0.5 cc. AcOH gave colorless crystals, m. 126-7°; the free base dissolved with heating in concentrated HCl on the steam bath, decolorized, and cooled deposited the  $\bar{\text{HCl}}$  salt, colorless transparent plates, m. 168-73°; turned lemon-yellow after several days.

L38 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1956:12242 HCAPLUS

DOCUMENT NUMBER:

50:12242

ORIGINAL REFERENCE NO.: 50:2534d-i,2535a-i,2536a-b

TITLE:

The preparation of substituted hydrazines. I.

Alkylhydrazines via alkylsydnones

AUTHOR(S):

Fugger, Joseph; Tien, Jack M.; Hunsberger, I. Moyer

Antioch Coll., Yellow Springs, O.

CORPORATE SOURCE: SOURCE:

Journal of the American Chemical Society (1955

), 77, 1843-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable CASREACT 50:12242

OTHER SOURCE(S):

3182-82-9, Glycine, N-butyl-, hydrochloride 56676-69-8,

Glycine, N-hexyl-, hydrochloride

(preparation of)

3182-82-9 HCAPLUS RN

Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

 $n-BuNH-CH_2-CO_2H$ 

● HCl

56676-69-8 HCAPLUS RN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME) CN

 $Me^- (CH_2)_5 - NH^- CH_2 - CO_2H$ 

HCl

The conversion of an alkylamine to an alkylhydrazine via the corresponding AΒ N-alkylglycine, N-nitroso-N-alkylglycine, and N-alkylsydnone is shown to constitute an acceptable preparative method in the cases of PhCH2NHNH2

(I), BuNHNH2 (II), and C6H13NHNH2 (III). The infrared spectra of  ${\tt N-benzyl sydnone\ (IV)\,,\ N-butyl sydnone\ (V)\,,\ and\ N-hexyl sydnone\ (VI)\ are}$ presented. ClCH2CO2Et (122 g.) and 214 g. PhCH2NH2 in 1 l. C6H6 refluxed 5 hrs. with stirring, the mixture filtered, the filtrate distilled to leave 154 g. PhCH2NHCH2CO2Et, yellow oil, the residue filtered, the crude ester added dropwise with stirring during 15 min. to 63.6 g. NaOH in 300 cc. H2O, the yellow solution refluxed 45 min. washed with Et2O, and acidified with concentrated HCl to pH 2, the resulting white suspension of PhCH2NHCH2CO2H treated at 0° with stirring during 0.5 hr. with 55.2 g. NaNO2 in 100 cc. cold H2O, the mixture stirred 2 hrs., brought to pH 2 with concentrated HCl, refrigerated 1 hr., and filtered, and the filter residue dried in vacuo over KOH yielded 139 g. crude PhCH2N(NO)CH2CO2H (VII). The VII heated 5 hrs. with stirring on the steam bath with 685 cc. Ac20, the resulting dark red solution filtered, and the filtrate evaporated in vacuo yielded 115 g. crude IV, red-brown oil, which solidified in an ice bath on scratching. The crude IV heated 4.5 hrs. on a steam bath with 1 l. 1:1 HCl, the red solution filtered, the clear filtrate concentrated to less than

100

cc. and filtered, and the residual crude I.HCl (56.8 g.) recrystd. twice from boiling EtOH yielded 14.6 g. pure I.HCl, m. 108-10.5°; and from mother liquor an addnl. 6.1 g. I.HCl. BrCH2CO2Et (68 cc.) in 100 cc. C6H6 added portionwise with swirling and cooling to 120 cc. BuNH2 in 300 cc., the mixture refluxed 2 hrs. on a steam bath, cooled, and filtered, the residual HBr salt (59 g.) washed with 80 cc. C6H6, the combined filtrate and washing concentrated in vacuo until white fumes appeared, the residue refluxed 25 min. with 28 g. NaOH in 120 cc. H2O, the cooled alkaline solution extracted with Et2O, the aqueous layer acidified with cooling to pH 2 with

 $ext{HCl}$ , and the mixture refrigerated and concentrated consecutively yielded 68.9 g.

crude BuNHCH2CO2H.HCl (VIII).HCl, snow-white needles and plates. Crude VIII.HCl (1 g.) in 10 cc. concentrated HCl warmed slightly on the steam bath and

filtered, the filtrate refrigerated, and this process repeated 3 times gave pure VIII.HCl, m. 204-5°. C6H13NH2 and BrCH2CO2Et gave in exactly the same manner crude C6H13NHCH2CO2H.HCl (IX.HCl); the alkaline polytical

of the IX.HCl swirled with cooling with 90 cc. concentrated HCl and 100 g. chopped ice precipitated immediately 81.0 g. IX.HCl, tiny yellowish white

refrigeration of the mother liquor gave an addnl. 4.8 g. IX.HCl. Crude IX.HCl (1 g.) in 10 cc. H2O treated with 1 cc. concentrated HCl, and the resulting precipitate treated 3 times in the same manner gave pure IX.HCl, snow-white flakes, m. 210-17°. Crude IX.HCl (1 g.) recrystd. from 20 cc. 1:1 MeOH-Me2CO or 40 cc. glacial AcOH gave the pure salt. VIII.HCl (78.0 g.) in 300 cc. H2O treated during 0.5 hr. at -4 to -5° with 37.5 g. NaNO2 in 100 cc. H2O, the mixture stirred 2 hrs., the oily bottom layer drawn off and dissolved in Et2O, and the solution filtered, dried, and evaporated gave 62.0 g. crude BuN(NO)CH2CO2H (X), yellow granular powder. Crude X (8.0 g.) crystallized from a small amount Et2O gave 4.53 g. nearly

white

granular solid, m. 60-2°, which recrystd. from aqueous EtOH or Et2O-petr. ether gave pure X, long snow-white flakes, m. 61-2°. An alkaline solution of IX prepared from 0.60 mole BrCH2CO2Et, cooled, treated

with stirring with 49.7 g. NaNO2 in 100 cc. H2O in 1 portion followed dropwise during 1.25 hrs. by 90 cc. concentrated HCl diluted with 50 g. ice, stirred 1

and adjusted with concentrated HCl to pH 2.0, the resulting brown oily top layer  $\,$ 

of crude C6H13N(NO)CH2CO2H (XI), (74.8 g.) allowed to stand, and the solidified yellow granular powder recrystd. from Et2O and then aqueous EtOH or petr. ether-Et2O gave pure XI, long white flakes, m. 79-80°. Crude X (40 g.) in 236 cc. Ac2O heated 3 hrs. on the steam bath, the mixture kept 1 day at room temperature, and the excess Ac2O distilled off gave 33 g. crude V; an

8-g. sample distilled yielded 4.5 g. pure V, pale yellow oil, b2 165-7°. X (0.362 mole) heated 3 hrs. with only 1.09 moles Ac2O gave nearly identical results. Crude yellow-white XI prepared from 0.20 mole BrCH2CO2Et dissolved in Et2O, the extract dried over Na2SO4, treated with 190 cc. Ac2O, kept 1 day at room temperature, and evaporated on the steam

the residual oil refluxed 3 hrs., the excess Ac20 removed in vacuo, and the clear brown oil dried in vacuo over KOH and P205 yielded 23 g. crude VI, which on distillation yielded 18 g. pure VI, b0.43 170-6° (redistd., b0.09 141-3°). XI (0.334 mole) dissolved in 1.14 moles warm AcOH, and the brown solution heated 2 hrs. on the steam bath after standing overnight yielded 93% VI. Crude V (40.5 g.) mixed with 80 cc. concentrated

the mixture heated 2 hrs. on the steam bath, cooled to room temperature, treated

with 20 cc. concentrated HCl, refrigerated overnight, treated with dry HCl to beginning crystallization, refrigerated again, and filtered, the residue washed with 1:1 MeOH-Et2O to yield 22 g. nearly white transparent needles, the filtrate decolorized with Norit A, saturated below 0° with dry HCl, refrigerated several days, neutralized with solid Na2CO3, and extracted with Et2O, a part of the extract treated with dry HCl, and the white precipitate

off gave II.HCl; the remainder of the extract treated in EtOH with (CO2H)2 yielded the oxalate of II. Distilled V (4.4 g.) heated 2.5 hrs. with concentrated

HCl, the yellow solution treated after 2 hrs. with an addnl. 10 cc. HCl, and the solution cooled and saturated with dry HCl yielded 3.1 g. II.HCl, thin white

plates, m. 149-54°. II.HCl (3.0 g.) treated with 15 cc. 25% aqueous Na2CO3, the alkaline mixture extracted with Et2O, and the extract distilled gave 1.0 g. V,

colorless liquid with an amine odor, b20 82-5°. Crude VI.HCl (40.7 g.) and 80 cc. concentrated HCl heated 2 hrs. on the steam bath, the mixture treated with an addnl. 30 cc. HCl and refrigerated, the dark brown cake dissolved in about 150 cc. H2O, and the solution heated a few min. on the steam bath with about 5 g. Norit, filtered hot, and cooled deposited 19.8 g. III.HCl, fine transparent needles; the mother liquor treated with (CO2H)2 in EtOH gave 18.0 g. III oxalate. The alkaline solution of the Na salt of IX from 0.60 mole BrCH2CO2Et treated below 0° with 37.2 g. NaNO2 in 120 cc. H2O in 1 portion, the mixture allowed to stand 0.5 hr., treated with 100 cc. concentrated HCl containing 50 g. crushed ice, stirred 1 hr., and acted

with Et20, and the Et20 evaporated gave a residue of 88.7 g. XI. XI (83.7 g.) heated 2 hrs. on the steam bath with 126 cc. Ac20, the excess Ac20 removed gave 81.5 g. crude VI. Crude VI (64 g.) heated 2 hrs. on a steam bath with 110 cc. concentrated HCl, cooled, neutralized with 25% aqueous NaOH, saturated with

K2CO3, and extracted 8 times with Et2O, the extract dried with K2CO, and added to

76 g. (CO2H)2 in 400 cc. 95% EtOH, the mixture allowed to stand overnight, and the yellowish solid filtered off and dried yielded 55.5 g. crude III.(CO2H)2. Crude III.(CO2H)2 (1.0 g.) recrystd. from 25 cc. hot 9:1 MeOH-EtOH yielded 410 mg. fluffy flakes, m. 171-2°; a 94-mg. sample in 5 cc. hot MeOH evaporated slowly at room temperature yielded 64 mg. large white

needles, m. 173-3.5°; this material dissolved in 5 cc. hot 4; 1 MeOH-EtOH, the solution filtered, and the filtrate poured into a sintered glass funnel gave 26 mg. pure III.(CO2H)2, transparent needles, m. 174.5-5.5°. II.HCl dissolved in 150-200 cc. H2O, neutralized with 30% aqueous NaOH in portions, saturated with solid K2CO3, and extracted with

extract dried over K2CO3 and added to 54 g. (CO2H)2 in 320 cc. 95% EtOH, the mixture allowed to stand overnight and filtered to give 18.5 g. crude salt, the mother liquor of the original II.HCl treated in the same manner to give an addnl. 6.3 g. oxalate, and the solid material combined gave 24.8 g. crude II.(CO2H)2. Crude II.(CO2H)2 (1 g.) recrystd. from 60 cc. hot 9:1 MeOH-EtOH yielded 420 mg. pure material, fine snow white needles; a sample (180 mg.) recrystd. from 20 cc. of the same solvent yielded 144 mg. pure material, white needles, m. 164-5°.

#### => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:19:19 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 28, 2004 (20040528/UP).

=>

41 1

145

06/03/2004

=> fil lreg

FILE 'LREGISTRY' ENTERED AT 08:16:10 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

LREGISTRY IS A STATIC LEARNING FILE

=> fil reg

FILE 'REGISTRY' ENTERED AT 08:16:12 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1 DICTIONARY FILE UPDATES: 2 JUN 2004 HIGHEST RN 688737-01-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:16:29 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

# => fil zcaplus

FILE 'ZCAPLUS' ENTERED AT 08:16:33 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 3 Jun 2004 VOL 140 ISS 23 FILE LAST UPDATED: 2 Jun 2004 (20040602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:16:39 ON 03 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

R15 unsubstituted
alkyl group FILE CONTAINS CURRENT INFORMATION. LAST RELOADED: May 28, 2004 (20040528/UP). => d que 138 L1 ( 1) SEA FILE=HCAPLUS ABB=ON PLU=ON (DURDEN, D? AND DAVIS, B? AND DYCK, L? AND LIU, Y? AND BOULTON, A? AND PATERSON, I?)/AU  $L_2$ SEL PLU=ON L1 1 RN : 103 TERMS compounds indexed for application L3 103) SEA FILE=REGISTRY ABB=ON PLU=ON L2 L4SCR 1518 L5 SCR 2050 2052 2043 Ь6 SCR 1526 L7SCR 1235 L8 STR CH\script CH3  $\mathtt{CH}^{\swarrow}\mathtt{Et}$ H3C-\langle C-\langle CH3 @9 10 @11 12 13 @14 15

H3C~~C~~Et 16 @17 18

```
REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
VAR G4=H/CH3
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

no substitutions

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

```
STEREO ATTRIBUTES: NONE
L9
                 SCR 963
        3584468) SEA FILE=REGISTRY ABB=ON PLU=ON N=1 NOT ((P/ELS OR SI/ELS)
L10 (
                OR (TIS OR MNS OR AYS OR PMS)/CI OR SEQUENCE/FS)
L11 (
            526) SEA FILE=REGISTRY SUB=L10 (SSS FUL) ((L4 AND L6 AND L7 AND L9)
                NOT L5) AND L8
             37) SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT (?NITRILE? OR
L12 (
                 ?PHOSPHONIC? OR ?AMINE? OR ?PROPENOIC? OR ?BROMO?)/CNS
L13 (
              2) SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND (C6 H13 N O2) /MF AND
                 (?GLYCINE? AND ?METHYLETHYL? AND ?METHYL?)/CNS
L14 (
             39) SEA FILE=REGISTRY ABB=ON PLU=ON L13 OR L12
L15 (
             16) SEA FILE=REGISTRY ABB=ON PLU=ON (16217-35-9/CRN OR 244189-98-
                8/CRN OR 244189-99-9/CRN OR 244190-00-9/CRN OR 244190-01-0/CRN
                OR 244190-02-1/CRN OR 244190-03-2/CRN OR 244190-04-3/CRN OR
                27453-30-1/CRN OR 31044-47-0/CRN OR 3183-21-9/CRN OR 3183-22-0/
                CRN OR 41331-10-6/CRN OR 42313-51-9/CRN)
L16 (
                                                                  set contains compoun named in application
             41) SEA FILE=REGISTRY ABB=ON PLU=ON L14 OR L15
L17
                STR
```

8
2 CH34
CH^CH3 CH^Et H3C^CC^CH3
CH^ACH3
CH^ET H3C^CC^CH3
Ak N C
3 || 0
7

H3C~~ C~~ Et 16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E3 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 1

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

```
L18
```

STR

```
2 4 CH\CH3 CH\Et H3C\C\CH3
1 Ak N C C C CH3
3 || 0
7
```

H3C~~C~~Et 16 @17 18

REP G1=(1-3) CH2
VAR G2=CH2/9/11/14/17
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E2 RC AT 3
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X17 C AT 3

#### GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 17

			remove qua
	ATTRIBUTES: NONE		1)40
L19 (	295)SEA FILE=REGISTRY	SUB=L11 (SSS FU)	$(L17 \text{ OR } L18)$ $\sim 5 $
L20 (	976)SEA FILE=HCAPLUS A	ABB=ON PL <del>U=ON</del>	
L21 (	5)SEA FILE=REGISTRY	ABB=ON PLU=ON	(58482-93-2 OR 42313-51-9 OR
	3338-22-5 OR 3183-	-22-0 OR 3183-23	1-9)/RN
L22 (	36)SEA FILE=REGISTRY	ABB=ON PLU=ON	L16 NOT L21
L23 (	34)SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L22
L24 (	28) SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L23 AND (PY<1999 OR AY<1999
	OR PRY<1999)		(1112333 OK A1(1333
L25 (	83) SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L21
L26 (	5)SEA FILE=HCAPLUS A		L24 AND L25
L27 (	28) SEA FILE=HCAPLUS A		L26 OR L24
L28 (	24)SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L20 AND L27
L29	28 SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L27 OR L28
L32	5 SEA FILE≃HCAPLUS A	ABB=ON PLU=ON	(58482-93-2? OR 42313-51-9?)
	(L) (BIOL OR USES)	/RL	12313 31 7.
L33	5 SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L32 AND (PY<1999 OR AY<1999
	OR PRY<1999)		(-1 (1)))
L34	14 SEA FILE=HCAPLUS A	ABB=ON PLU=ON	42313-51-9?
L35	14 SEA FILE=HCAPLUS A		L34 AND (PY<1999 OR AY<1999
	OR PRY<1999)		(-1,12)
L37	1 SEA FILE=HCAPLUS A	ABB=ON PLU=ON	L35 AND (A61K?)/ICM
L38	33 SEA FILE=HCAPLUS A		L37 OR L33 OR L29
			· === + ==>

=> d 138 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:y

L38 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

```
Reyes 09/646,110
ACCESSION NUMBER:
                         1999:626163 HCAPLUS
                                                            Applicants
DOCUMENT NUMBER:
                         131:243589
TITLE:
                        Aliphatic amino carboxylic and amin
                        amino nitriles, and amino tetrazole
                        rescue agents
INVENTOR (S):
                        Paterson, I. Alick; Dyck, Lilian E.
                        Liu, Ya-Dong; Durden, David A.; Boul
PATENT ASSIGNEE(S):
                        University of Saskatchewan Technolog
                        The Canada Trust Company
SOURCE:
                        PCT Int. Appl., 52 pp.
                        CODEN: PIXXD2
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
    PATENT NO.
                     KIND DATE
                                          APPLICATION NO.
                                                           DATE
                     ----
     ------
                           _____
                                          ------
                                                           -----
    WO 9948858
                     A2
                           19990930
                                          WO 1999-CA250
                                                           19990325 <--
    WO 9948858
                      A3
                           20000120
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
            DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
            JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,
            MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
            TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
            MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
            ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
            CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    CA 2325943
                      AA
                           19990930
                                         CA 1999-2325943 19990325 <--
    AU 9928240
                      A1
                           19991018
                                          AU 1999-28240
                                                           19990325 <--
    AU 767098
                      В2
                           20031030
    TR 200002756
                      T2
                           20001221
                                          TR 2000-20000275619990325 <--
    EP 1064254
                      A2
                           20010103
                                          EP 1999-908728 19990325 <--
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
```

OTHER SOURCE(S): MARPAT 131:243589 IT 3338-22-5P 31044-48-1P 41331-11-7P

IE, SI, LT, LV, FI, RO

20011016

20020312

20010507

20000925

Α

T2

Α

Α

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

BR 1999-9103

ZA 2000-4988

NO 2000-4774

US 1998-79488P

US 1998-79489P

WO 1999-CA250

JP 2000-537843

Ρ

19990325 <--

19990325 <--

20000919 <--

20000925 <--

19980326 <--

P 19980326 <--

W 19990325

RN 3338-22-5 HCAPLUS

BR 9909103

JP 2002507591

ZA 2000004988

NO 2000004774

PRIORITY APPLN. INFO.:

CN Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H ● HCl RN31044-48-1 HCAPLUS CN $\beta$ -Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)  $MeO-C-CH_2-CH_2-NH-(CH_2)_5-Me$ HC1 RN41331-11-7 HCAPLUS CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)  $Me^{-(CH_2)_5-NH-CH_2-CH_2-CO_2H}$ IT 3183-21-9P 3183-22-0P 3183-23-1P 16217-35-9P 27453-30-1P 31044-47-0P 40870-77-7P 41331-10-6P 42313-51-9P 56676-69-8P 244189-67-1P 244189-68-2P 244189-69-3P 244189-70-6P 244189-71-7P 244189-72-8P 244189-73-9P 244189-74-0P 244189-75-1P 244189-98-8P 244189-99-9P 244190-00-9P 244190-01-0P 244190-02-1P 244190-03-2P 244190-04-3P 244190-26-9P 244190-27-0P 244190-28-1P 244190-31-6P 244190-32-7P 244190-33-8P 244190-34-9P

244190-37-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aliphatic amino carboxylic and amino phosphonic acids, amino nitriles, and amino tetrazoles as cellular rescue agents)

RN 3183-21-9 HCAPLUS

CN Glycine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H

RN 3183-22-0 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 3183-23-1 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 16217-35-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)

$$i-PrNH-CH_2-CH_2-CO_2H$$

RN 27453-30-1 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ | & || \\ \text{i-Pr-N-CH}_2\text{--CH}_2\text{--C-OMe} \end{array}$$

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{O} & \\ || & \\ \text{MeO-C-CH}_2\text{--CH}_2\text{--NH--(CH}_2)}_5\text{--Me} \end{array}$$

RN 40870-77-7 HCAPLUS

CN β-Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

## HCl

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^-(CH_2)_5 - NH - CH_2 - CO_2H$ 

RN 42313-51-9 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

 $Me^- (CH_2)_5 - NH - CH_2 - CO_2H$ 

# ● HCl

RN 244189-67-1 HCAPLUS CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### HCl

RN 244189-68-2 HCAPLUS

CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \\ \text{HN} \\ \\ \text{CO}_2 \text{H} \end{array}$$

● HCl

RN 244189-69-3 HCAPLUS 
CN  $\beta$ -Alanine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Me^{(CH_2)_4}$$
  $S$   $Me$   $HN$   $CO_2H$ 

● HCl

RN 244189-70-6 HCAPLUS CN  $\beta$ -Alanine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

 $i-PrNH-CH_2-CH_2-CO_2H$ 

● HCl

RN 244189-71-7 HCAPLUS CN Glycine, N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME) Absolute stereochemistry.

Me 
$$(CH_2)_4$$
 R Me HN  $CO_2H$ 

● HCl

RN 244189-72-8 HCAPLUS CN Glycine, N-[(1S)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME) Absolute stereochemistry.

● HCl

RN 244189-73-9 HCAPLUS
CN β-Alanine, N-methyl-N-(1

CN  $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 244189-74-0 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} & \text{Me} \\ \text{Me} & \text{N} \\ \text{Me} & \text{OMe} \end{array}$$

● HCl

RN 244189-75-1 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### ● HCl

RN 244189-98-8 HCAPLUS CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244189-99-9 HCAPLUS CN  $\beta$ -Alanine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} & \text{Me} \\ \text{Me} & \text{HN} \\ \end{array}$$

RN 244190-00-9 HCAPLUS CN  $\beta$ -Alanine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$^{(CH_2)_4}$$
  $^{Me}$   $^{HN}$   $^{CO_2H}$ 

RN 244190-01-0 HCAPLUS CN Glycine, N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-02-1 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me 
$$(CH_2)_4$$
 S Me  $HN$   $CO_2H$ 

RN 244190-03-2 HCAPLUS

CN  $\beta$ -Alanine, N-methyl-N-[(1R)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{(CH}_2)_4 \\ \text{Me} \\ \\ \text{N} \\ \\ \text{O} \end{array} \qquad \begin{array}{c} \text{OMe} \\ \\ \\ \text{O} \end{array}$$

RN 244190-04-3 HCAPLUS

CN β-Alanine, N-methyl-N-[(1R)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{(CH}_2)_4 & \text{Me} \\ \\ \text{Me} & \\ \\ \text{N} & \\ \\ \text{CO}_2\text{H} \end{array}$$

RN 244190-26-9 HCAPLUS

CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me 
$$(CH_2)_4$$
 S Me  $CO_2H$ 

RN 244190-27-0 HCAPLUS

CN Glycine, N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-28-1 HCAPLUS

CN Glycine, N-methyl-N-[(1S)-1-methylhexyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 244190-31-6 HCAPLUS

CN β-Alanine, N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 244190-32-7 HCAPLUS

CN Glycine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & | & || \\ \text{i-Pr-N-CH}_2\text{--C-OMe} \end{array}$$

RN 244190-33-8 HCAPLUS

CN Glycine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

RN 244190-34-9 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \text{Me} \\ \parallel & \parallel \\ \text{MeO-C-CH}_2\text{-CH}_2\text{-N-(CH}_2)} \\ \text{5-Me} \end{array}$$

RN244190-37-2 HCAPLUS CN  $\beta$ -Alanine, N-hexyl-N-methyl- (9CI) (CA INDEX NAME)

Мe  ${\rm HO_2C-CH_2-CH_2-N-(CH_2)_5-Me}$ 

AΒ Tile compds. R1R2R3CNR4(CH2)nX [R1 = Me(CH2)n (n = 1-16), alkenyl,alkynyl, alkoxy, alkylthio, alkylsulfinyl; R2 = H, Me, Et; R3, R4 = H, Me; X = CO2H or carbalkoxy, cyano, PO3H2 or phosphonate ester, 5-tetrazolyl] or their pharmaceutically acceptable salts were prepared Thus, Me 3-(1-hexylamino)propionate hydrochloride was prepared by addition reaction of 1-hexylamine with Me acrylate and shown to have antiapoptotic activity at 10-6 M.

=> d 138 ibib hitstr abs 2-YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y) /N:y

YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

L38 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1998:675926 HCAPLUS

DOCUMENT NUMBER:

130:3527

TITLE:

Selective addition of amines to methyl acrylate in

presence of alumina

AUTHOR (S):

Suzuki, Yoshitada; Murakami, Shunsuke; Kodomari,

Mitsuo

CORPORATE SOURCE:

Department of Industrial Chemistry, Faculty of Engineering, Shibaura Institute of Technology,

Minato-ku, Tokyo, 108-8548, Japan

SOURCE:

Nippon Kagaku Kaishi (1998), (10), 664-669

CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER:

Nippon Kagakkai

DOCUMENT TYPE:

Journal Japanese

LANGUAGE:

31044-47-0P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(selective addition of amines to Me acrylate in presence of alumina)

RN31044-47-0 HCAPLUS

CNβ-Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

 $-C-CH_2-CH_2-NH-(CH_2)_5-Me$ 

AB1 The Michael type addition of primary amines to Me acrylate in benzene was accelerated by alumina, and monoadducts were selectively obtained in high yield. The reaction in benzene did not proceed without alumina. yields of adducts were dependent on the structure of amines; the monoadducts were obtained in high yield (77-91% yield) when linear amines were used, and in the case of branched or bulky primary amines and secondary amines, the yields were decreased compared to the linear ones. In the addition of diamines to Me acrylate, only an amino group on 1 side of the diamines added to Me acrylate to give the monoadducts selectively, and

AB Substituted amines R1NR2R3 [R1 = acidic group containing at least one OH; R2 = H, Me, PhCH2, R1, R3; R3 = CR4R5CHR6R7; R2R3N = heterocyclyl; R4, R5 = H, C1-6 alkyl, (un)substituted aryl; R6, R7 = R4, R5, OH, C1-6 alkoxy, aryloxy, halo, SH, thioalkyl, mono- or dialkylamino, or, when R6 = H, R7 can be N(CH2CO2H)2] were dealkylated by heating at 250-400° in aqueous alkali, using at least the stoichiometric amount of alkali needed to neutralize the acidic OH groups, to give R1R2NH with removal of R3 groups as alkenes. The process is useful for preparation of valuable amino acids, e.g., glycine, sarcosine, iminodiacetic acid, and aminomethylphosphonic acid. Thus, a solution of 0.038 mol Me2CHNMeCH2CO2H in H2O containing 0.076

mol

NaOH was heated at  $300^{\circ}$  in an Monel autoclave to give 71% sarcosine.

L38 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1986:462332 HCAPLUS

DOCUMENT NUMBER:

105:62332

TITLE:

Ę

Surface treatment of zinc base materials

INVENTOR (S):

Kurihara, Masao; Kimata, Shizuro; Imura, Hideaki;

Naruse, Naohiko

PATENT ASSIGNEE(S):

Toa Gosei Chemical Industry Co., Ltd., Japan

SOURCE:

Jpn. Tokkyo Koho, 9 pp.

BOOKCE

CODEN: JAXXAD

DOCUMENT TYPE:

LANGUAGE:

Patent Japanese

FAMILY ACC. NUM. COUNT: 1

FAMILI ACC. NOM. COUNT

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60056225	B4	19851209	JP 1978-102938	19780825 <
JP 55031417	A2	19800305		
PRIORITY APPLN. INFO.	:		JP 1978-102938	19780825 <

IT 41331-11-7 41421-76-5

41331-11-7 41421-76-RL: USES (Uses)

(pretreatment by aqueous alkalies and, of zinc, for coating with powdered epoxy resin)

RN 41331-11-7 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_5-NH-CH_2-CH_2-CO_2H}$ 

RN 41421-76-5 HCAPLUS

CN Butanoic acid, 4-(dodecylamino)- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_{11}-NH^{-(CH_2)_3}-CO_2H}$ 

AB Surfaces of zinc are treated with aqueous alkali hydroxide and aqueous solns. of

RNHCnH2nCO2H (R = >C6 saturated or unsatd. aliphatic hydrocarbyl groups, n > 2) or H halide solns. and coated. Thus, Zn-plated steel was degreased, treated with 6% aqueous KOH, immersed 5 min at 90° in 3% aqueous hexyl- $\beta$ -aminopropionic acid, dried, electrostatically coated with a powdered epoxy resin, and baked to form a coating.

L38 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

```
1986:73067 HCAPLUS
ACCESSION NUMBER:
                          104:73067
DOCUMENT NUMBER:
                          Effect of surfactants on the formation of a metallic
TITLE:
                          film during metalizing of glass fibers
                          Ermakov, E. A.; Pantaev, V. A.
AUTHOR (S):
                          Kalinin. Gos. Univ., Kalinin, USSR
Khim. Poverkhn.-Akt. Veshchestv Kompleksonov (
CORPORATE SOURCE:
SOURCE:
                          1984), 107-10. Editor(s): Gorelov, I. P.
                          Kalinin. Gos. Univ.: Kalinin, USSR.
                          CODEN: 54JOAA
DOCUMENT TYPE:
                          Conference
LANGUAGE:
                          Russian
IT
     41331-11-7
     RL: USES (Uses)
         (surfactant, in electroless copper coating of glass fibers, film d. and
        structure in relation to)
RN
     41331-11-7 HCAPLUS
     β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)
CN
Me^{-(CH_2)}_{5}-NH^{-CH_2}-CH_2-CO_2H
     The effect of surfactants, i.e. Na alkylsulfates and alkyl-\beta-alanine
AB
     on the formation of a metal film during electroless Cu coating of glass
     fibers was studied. Elec. resistance of the fibers metalized without
     surfactants was substantially higher than that of samples prepared using the
     surfactants, which was associated with the difference in the Cu film surface
     defectiveness. Coatings obtained using the surfactants were distinguished
     by the fine-crystalline structure, whereas without them, coarser crystallites
     formed, and the coating was less dense. The best results in preparing dense
     coatings with fine-grained structure were observed when electroless bath
     contained Na undecylsulfate [1072-24-8] and N-hexyl-β-alanine
     41331-11-7].
L38 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                          1986:24719 HCAPLUS
DOCUMENT NUMBER:
                           104:24719
                          Effect of inorganic salts of tin and palladium on
TITLE:
                           colloidal-chemical properties of surfactants
                          Voronchikhina, L. I.; Pavlova, L. A.
AUTHOR (S):
                          Kalinin. Gos. Univ., Kalinin, USSR
Khim. Poverkhn.-Akt. Veshchestv Kompleksonov (
CORPORATE SOURCE:
SOURCE:
                          1984), 88-92. Editor(s): Gorelov, I. P. Kalinin. Gos. Univ.: Kalinin, USSR.
                           CODEN: 54JOAA
DOCUMENT TYPE:
                           Conference
                          Russian
LANGUAGE:
     41331-11-7
     RL: PEP (Physical, engineering or chemical process); PRP (Properties);
     PROC (Process)
         (surface activity of, in presence of tin or palladium chlorides)
RN
     41331-11-7 HCAPLUS
     β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)
```

 ${\tt Me-(CH_2)_5-NH-CH_2-CH_2-CO_2H}$ 

AB The behavior of colloidal solns. of surfactants (amphoteric

N-dodecyl-N,N-dimethyl- $\alpha$ -betain and N-ketyl- $\beta$ -alanine; anionic Na cetyl sulfate and Na undecyl sulfate and cationic decylpyridinium chloride and dodecylbenzyldimethylammonium chloride) was studied in the presence of SnCl2 and PdCl2. The saturated adlayer formation, critical micellization concentration, and surface tension were determined At < 0.5M SnCl2 and

PdCl2 in solns., surface activity of the amphoteric and anionic surfactants increases significantly. The cationic surfactants are unstable in the presence of > 0.05M surfactants.

L38 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1980:147180 HCAPLUS

DOCUMENT NUMBER:

92:147180

TITLE:

Cation-binding cyclic peptides with lipophilic tails

AUTHOR(S):

Deber, C. M.; Adawadkar, P. D.

CORPORATE SOURCE:

Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8,

Can.

SOURCE:

Biopolymers (1979), 18(10), 2375-96

CODEN: BIPMAA; ISSN: 0006-3525

DOCUMENT TYPE:

Journal English

LANGUAGE:

20933-56-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and esterification of, with benzyl alc.)

RN 20933-56-6 HCAPLUS

CN Glycine, N-decyl- (8CI, 9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_9-NH-CH_2-CO_2H}$ 

IT 41331-10-6P

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_5-NH-CH_2-CO_2H}$ 

AB Cyclo[Glu(OCH2Ph)-Sar-Gly-NRCH2CO]2 (I; Sar = NMeCH2CO, R = Me) was prepared by coupling BOC-Glu(OCH2Ph)-Sar-Gly-Sar-OH (BOC = Me3CO2C) to H-Glu(OCH2Ph)-Sar-Gly-Sar-OH by the mixed anhydride method, esterifying the resulting octapeptide with HOC6H4NO2-p, BOC-deblocking the resulting p-nitrophenyl ester with HCl, and cyclizing the resulting H-[Glu(OCH2Ph)-Sar-Gly-Sar]2-OC6H4NO2-p in DMF/pyridine at high dilution I [R = decyl (II), hexyl, cyclohexyl], cyclo[Glu(OCH2Ph)-Sar-Gly-Sar-Glu(OCH2PH)-Sar-Gly-NR1CH2CO]2 (R1 = decyl), and cyclo(Phe-Sar-Gly-Sar)2 were also prepared, and the above α-benzyl esters were converted to the free acids. Proton and 13C NMR data showed that I with a mixture of cis/trans peptide bond conformers were converted to the C2-sym. all-trans conformers upon complexation with Ca2+. II mediated the transport of cations across a thick-liquid membrane with the following selectivity: Ca2+ > Na+ > K+ > Mn2+ > Cu2+ > Mg2+ > Co2+ > Zn2+.

L38 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1977:135270 HCAPLUS

DOCUMENT NUMBER:

86:135270

TITLE:

Facilitated diffusion of amino acids across

bimolecular lipid membranes as a model for selective accumulation of amino acids in a primordial protocell

Stillwell, William

CORPORATE SOURCE:

Dep. Biophys., Michigan State Univ., East Lansing, MI,

USA

SOURCE:

BioSystems (1976), 8(3), 111-17 CODEN: BSYMBO; ISSN: 0303-2647

DOCUMENT TYPE:

Journal

LANGUAGE:

AUTHOR(S):

English

627-01-0 3182-81-8 41331-10-6 50997-13-2

RL: PEP (Physical, engineering or chemical process); PROC (Process) (diffusion of, across lipid membrane)

RN627-01-0 HCAPLUS

Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

EtNH-CH2-CO2H

3182-81-8 HCAPLUS RN

Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME) CN

n-BuNH-CH2-CO2H

41331-10-6 HCAPLUS RN

CNGlycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-}(CH_2)_{5}-NH-CH_2-CO_2H$ 

50997-13-2 HCAPLUS RN

Glycine, N-nonyl- (9CI) (CA INDEX NAME) CN

 $Me^-(CH_2)_8-NH-CH_2-CO_2H$ 

A simple transport system for the uptake of amino acids into lipid ABvesicles was studied as a model for the protocell. The rate of diffusion of amino acids across bimol. lipid membranes was greatly stimulated by water-soluble aldehydes. Even HCHO was an effective carrier, although pyridoxal was much more effective. Series of reduced amino acid imines of qlycine, lysine, and histidine were synthesized to measure the relative abilities of different aldehydes as carriers for amino acids. Comparison of partition coeffs. to the diffusion rates of the derivatized amino acids indicated that the more lipophilic derivs. are more readily diffused. This simple type of facilitated diffusion makes lipid vesicles an attractive model of the 1st primoridal cell.

L38 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1976:430029 HCAPLUS

DOCUMENT NUMBER:

85:30029

TITLE:

Oxidation of sarcosine and N-alkyl derivatives of

glycine by D-amino-acid oxidase

AUTHOR(S): Naoi, Makoto; Yaqi, Kunio

CORPORATE SOURCE:

Fac. Med., Univ. Nagoya, Nagoya, Japan Biochimica et Biophysica Acta (1976),

438(1), 61-70

CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE:

Journal English

LANGUAGE:

SOURCE:

627-01-0 3182-81-8 25303-14-4

35386-27-7 41331-10-6

RL: BIOL (Biological study)

L: BIOL (BIOlogical Study)

(amino acid oxidase specificity for)

RN 627-01-0 HCAPLUS

CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH2-CO2H

RN 3182-81-8 HCAPLUS

CN Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH2-CO2H

RN 25303-14-4 HCAPLUS

CN Glycine, N-propyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

 $n-PrNH-CH_2-CO_2H$ 

RN 35386-27-7 HCAPLUS

CN Glycine, N-pentyl- (6CI, 9CI) (CA INDEX NAME)

 $Me^- (CH_2)_4 - NH^- CH_2 - CO_2H$ 

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^-(CH_2)_5 - NH^-CH_2 - CO_2H$ 

AB Sarcosine was oxidized by D-amino acid oxidase (EC 1.4.3.3) to yield methylamine and glyoxylic acid. A series of N-alkyl glycines were also oxidized by this enzyme. N-acetyl- and N-phenylglycine inhibited the oxidase by competing with the substrate, whereas N-methyl-N-acetylglycine did not bind to the enzyme. This suggests the requirement of at least 1 unsubstituted H atom at the amino group of glycine for binding. The primary step in the reaction was the release of a proton from the substrate, indicating the formation of a substituted imino acid, which was spontaneously hydrolyzed to glyoxylic acid and an amine.

L38 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1975:514857 HCAPLUS

DOCUMENT NUMBER:

83:114857

TITLE:

Preparation of N-alkyl and N-arylglycines from glyoxylic acid using carbonylhydridoferrate as a

reducing agent

AUTHOR (S):

Watanabe, Yoshihisa; Shim, Sang Chul; Mitsudo, Takeaki; Yamashita, Masakazu; Takegami, Yoshinobu

CORPORATE SOURCE: SOURCE:

Fac. Eng., Kyoto Univ., Kyoto, Japan Chemistry Letters (1975), (7), 699-700

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE:

Journal English

LANGUAGE:

3182-82-9P 56676-69-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

3182-82-9 HCAPLUS RN

Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

n-BuNH-CH2-CO2H

● HCl

56676-69-8 HCAPLUS RN

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

 $Me^-(CH_2)_5-NH-CH_2-CO_2H$ 

● HCl

To Fe(CO)5 and alc. in KOH was added an amine, glyoxylic acid and EtOH and the mixture stirred 24 hr at room temperature. The precipitate was acidified with concentrate

HCl to give salts of glycines, RNHCH2CO2H·HCl (R = Me, Bu, hexyl, cyclohexyl, PhCH2, Ph, p-MeC6H4, p-MeOC6H4, p-ClC6H4, β-naphthyl.

L38 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1975:409540 HCAPLUS

DOCUMENT NUMBER:

83:9540

TITLE:

Alkyl 5-oxoalkanoates

INVENTOR(S):

Mueller, Werner

PATENT ASSIGNEE(S):

Farbwerke Hoechst A.-G. Ger. Offen., 11 pp.

SOURCE:

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2325160	A1	19741205	DE 1973-2325160	19730518 <
ZA 7402951	Α	19750528	ZA 1974-2951	19740508 <
IN 141915	Α	19770430	IN 1974-CA1033	19740509 <
NL 7406400	Α	19741120	NL 1974-6400	19740513 <
CH 593902	A	19771230	CH 1974-6689	19740515 <
IT 1012464	Α	19770310	IT 1974-22850	19740516 <

```
19741213
    FR 2229679
                       Α1
                                           FR 1974-17272
                                                            19740517 <--
                            19781117
    FR 2229679
                       В1
    JP 50030829
                       Α2
                            19750327
                                           JP 1974-54612
                                                            19740517 <--
    BE 815282
                       Α1
                            19741120
                                           BE 1974-144528
                                                            19740520 <--
    GB 1473184
                       Α
                            19770511
                                           GB 1974-22412
                                                            19740520 <--
PRIORITY APPLN. INFO.:
                                        DE 1973-2325160
                                                            19730518 <--
    42313-51-9
    RL: CAT (Catalyst use); USES (Uses)
        (catalyst, for ketone addition to alkyl acrylates)
RN
     42313-51-9 HCAPLUS
    β-Alanine, N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)
MeO-C-CH2-CH2-NHPr-i
    Fifteen RCOCHR1CH2CHR2CO2R3 [R = Me, Et, Bu, or Ph; R1 = H, Me, Pr, or Ph;
    or RR1 = (CH2)4; R2 = H or Me; R3 = C1-4 alkyl] or their mixts. were
    prepared by reaction of RCOCH2R1 with CH2:CR2CO2R3 in the presence of
     amines. Thus, Me2CO and CH2: CHCO2Me were autoclaved in the presence of
     aqueous Me2CHNH2 and BzOH at 180° to give 84.5% MeCO(CH2)3CO2Me and <
     10% (MeO2CCH2CH2) 2CHCOMe.
L38 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
                         1974:888 HCAPLUS
ACCESSION NUMBER:
                         80:888
DOCUMENT NUMBER:
                         Diffusion of glycine and N-substituted glycines across
TITLE:
                         bimolecular lipid membranes
AUTHOR (S):
                         Stillwell, William; Winter, Harry C.
                         Dep. Biochem., Pennsylvania State Univ., University
CORPORATE SOURCE:
                         Park, PA, USA
                         Biochemical and Biophysical Research Communications (
SOURCE:
                         1973), 54(4), 1437-43
                         CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE:
                         Journal
                         English
LANGUAGE:
     627-01-0 3182-81-8 41331-10-6
     50997-13-2
    RL: PEP (Physical, engineering or chemical process); PROC (Process)
        (diffusion of, across liposome)
RN
     627-01-0 HCAPLUS
    Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
CN
EtNH-CH2-CO2H
     3182-81-8 HCAPLUS
RN
     Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
n-BuNH-CH2-CO2H
    41331-10-6 HCAPLUS
RN
    Glycine, N-hexyl- (9CI) (CA INDEX NAME)
```

```
Me^{-(CH_2)_5-NH-CH_2-CO_2H}
```

RN 50997-13-2 HCAPLUS CN Glycine, N-nonyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}8^{-NH-CH_2-CO_2H}$ 

AB Free glycine diffused very slowly across synthetic bimol. lipid membranes, whereas several N-substituted derivs. of glycine penetrated the membranes more readily. Pyridoxal, formaldehyde, and acetaldehyde enhanced the diffusion of glycine across the membranes, presumably the result of imine formation between the aldehyde and the  $\alpha$ -amino group of glycine. Several N-substituted glycines were synthesized and their rates of efflux from liposomes were related to their H2O-CHCl3 partition coeffs. This is the 1st demonstration of carrier-mediated diffusion of amino acids across a bimol. lipid membrane.

L38 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1973:101277 HCAPLUS

DOCUMENT NUMBER:

78:101277

TITLE:

Synergistic combinations for inhibiting the attack of

alkaline solutions on alkali-sensitive substrates

INVENTOR(S):

Dupre, Jean; Booman, Keith A.

PATENT ASSIGNEE(S):

Rohm and Haas Co. U.S., 7 pp.

SOURCE:

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
US 3653095	A	19720404		US 1969-835906	19690618 <
GB 1320793	A	19730620		GB 1970-29430	19700617 <
PRIORITY APPLN.	INFO.:		US	1969-834499	19690618 <
			US	1969-835906	19690618 <

IT 1462-54-0 41331-10-6 41331-11-7

RL: USES (Uses)

(corrosion inhibition by, of alkaline solns.)

RN 1462-54-0 HCAPLUS

CN β-Alanine, N-dodecyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

```
Me^{-(CH_2)_{11}-NH-CH_2-CH_2-CO_2H}
```

RN 41331-10-6 HCAPLUS

CN Glycine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}_{5}-NH^{-CH_2}-CO_2H$ 

RN 41331-11-7 HCAPLUS

CN β-Alanine, N-hexyl- (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)_5-NH-CH_2-CH_2-CO_2H}$ 

AB During cleaning with an aqueous alkaline solution containing 0.1-10 weight % alkali,

materials (e.g. Al, Zn, Sn, Pb, their alloys, Si oxides and compds. containing Si oxides) which are sensitive to the alkaline attack are protected by a synergistic combination of:  $\geq 1$  metal ion (0.005M) such as Ba2+, Ca2+, and Sr2+ with  $\geq 1$  surface-active agent (0.5 weight %) selected from alkyl glycosides having a formula ROGmH, where G is a glycosyl radical, R is C6-16 alkyl connected to C-1 of the glycosyl radical through the O, and m = 1-4; or ethylene oxide adducts of the alkyl glycosides containing  $\leq 2$  ethylene oxide units per glycosyl radical; or amino carboxylic acids having C $\geq 10$  and metal salts of amino carboxylic acids (0.01-5 weight %). Optionally in certain and essentially in other applications, a H2O-soluble naphthalene derivative may be added to the synergistic combination.

L38 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1973:38037 HCAPLUS

DOCUMENT NUMBER:

78:38037

TITLE:

Potential hypotensive compounds. Substituted

3-aminopropionates and 3-aminopropionohydroxamic acids

AUTHOR(S):

Biggs, D. F.; Coutts, R. T.; Selley, M. L.; Towill, G.

Α.

CORPORATE SOURCE:

Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB,

Can.

SOURCE:

Journal of Pharmaceutical Sciences (1972),

61(11), 1739-45

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE:

LANGUAGE:

Journal English

IT 40870-77-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and hypotensive effect of)

RN 40870-77-7 HCAPLUS

CN  $\beta$ -Alanine, N-(1-methylethyl)-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

O || MeO-C-CH<sub>2</sub>-CH<sub>2</sub>-NHPr-i

#### ● HCl

Most of the 48 3-aminoproprionate esters studied were synthesized by addition of an amine across the  $\alpha,\beta$ -double bond of Me acrylate [96-33-3], Me methacrylate [80-62-6], or Me crotonate [18707-60-3], while the remainder were obtained by interaction of 1 mole of a 3-bromopropionic ester with 2 moles of the corresponding amine. Twenty-six 3-aminopropionohydroxamic acid hydrochlorides were prepared by treatment of the appropriate amino ester with hydroxylamine-HCl [5470-11-1] in MeOH. Many of the compds. such as 2-methyl-3-[(2-phenylethyl)amino]propanoic acid Me ester [6297-67-2], 3,3'-[(2-phenylethyl)imino]bispropanoic acid dimethyl ester [38129-46-3], N-{3-(hydroxyamino)-2-methyl-3-

oxopropyl]heptanaminium chloride [38129-47-4], and N-[3-(hydroxyamino)-3-oxopropyl]-2-(2-phenylethyl)benzeneethanaminium chloride [38202-84-5] possessed hypotensive properties but of very short duration.

2-Methyl-3-(octylamino)propanoic acid Me ester [29228-46-4] was the most active, and at 4 mg/kg i.v. decreased the blood pressure of rats by an average of 52% for 12 min. Some of the compds. were screened for their ability to protect mice against a lethal dose of diisopropylfluorophosphate [55-91-4], but none was active.

L38 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1971:75986 HCAPLUS

DOCUMENT NUMBER:

74:75986

TITLE:

Synthesis and properties of some hypotensive

N-alkylaminopropionic esters and N,N-

dialkylaminopropionic esters and their hydroxamic

acids

AUTHOR(S):

Coutts, Ronald T.; Hubbard, J. W.; Midha, Kamal K.;

Prasad, Kailash

CORPORATE SOURCE:

Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB,

Can.

SOURCE:

Journal of Pharmaceutical Sciences (1971),

60(1), 28-33

CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE:

Journal English

LANGUAGE:

10478-41-8P 31044-47-0P 31044-48-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 10478-41-8 HCAPLUS

CN β-Alanine, N-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

 $\mathtt{EtNH-CH_2-CH_2-CO_2H}$ 

RN 31044-47-0 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester (8CI, 9CI) (CA INDEX NAME)

$$MeO-C-CH_2-CH_2-NH-(CH_2)_5-Me$$

RN 31044-48-1 HCAPLUS

CN  $\beta$ -Alanine, N-hexyl-, methyl ester, hydrochloride (8CI, 9CI) (CA INDEX NAME)

## ● HCl

GI For diagram(s), see printed CA Issue.

AB Thirty-eight 3-(N-alkylamino) - and 3-(N,N-dialkylamino) propionic esters

(I), hydroxamic acids (II), carboxylic acids, and related compds. were synthesized and the majority of the esters and hydroxamic acids decreased the blood pressure of anesthetized cats, while the carboxylic acids were inactive. The esters were prepared by the interaction of methyl acrylate or methyl methacrylate and an appropriate amine. Some hindered amines did not react with the acrylate, and some esters hydrolyzed to the corresponding carboxylic acids when stored even for a short time. hydroxamic acids were prepared from the amino esters treated with hydroxylamine.

L38 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1970:445265 HCAPLUS

DOCUMENT NUMBER:

73:45265

TITLE:

Derivatives of substituted acetic acids. XXVIII.

Dialkylaminopropyl esters of  $\alpha$ naphthylheterylacetic acids

AUTHOR (S):

Mndzhoyan, A. L.; Badalyan, V. E.

CORPORATE SOURCE:

Inst. Tonkoi Org. Khim., Erevan, USSR Armyanskii Khimicheskii Zhurnal (1970),

SOURCE: 23(4), 258-67

CODEN: AYKZAN; ISSN: 0515-9628

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

IT 27453-30-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 27453-30-1 HCAPLUS

CN $\beta$ -Alanine, N-methyl-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ | & || \\ \text{i-Pr-N-CH}_2\text{--CH}_2\text{--C-OMe} \end{array}$$

AΒ A mixture of 0.5 mole R1R2NH, 0.5 mole CH2:CHC02Me, in 200 ml C6H6 refluxed for 6-8 hr (with iso-PrR2NH, the mixture was heated at 95° in a sealed tube 16-20 hr while with (iso-Pr)2NH similarly treated for 150 hr. to give R1R2NCH2CH2CO2Me (I). LiAlH4 reduction of (I) gave R1R2NCH2CH2CH2OH (II) which, in refluxing PhMe, reacted with  $\alpha\text{-C10H7CHClCOCl}$  (III) [from  $\alpha$ -C10H7CH(OH)CO2H (50.5 g) and refluxing SOCl2 (180 ml)] to give the corresponding  $\alpha$ -C10H7CHClCO2(CH2)3NR1R2 (IV). IV treated with an amine yielded the title  $\alpha$ -C10H7CHR3CO2(CH2)3NR1R2 (V). Thus a mixture of 0.025 mole IV, 0.05 mole piperidine, and 100 ml PhMe refluxed 6-8 hr gave 77% V (R1 = R2 = Me, R3 = piperidino), b3 228-30°. The morpholino analog was similarly prepared Approx. 150 new compds. and derivs. were reported.

L38 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1967:517255 HCAPLUS

DOCUMENT NUMBER:

67:117255

TITLE:

Preparation of N-substituted aspartic esters,  $\beta$ -amino esters, and their corresponding acids

Pfau, Michel

CORPORATE SOURCE:

Lab. Chim. Ecole Norm. Super., Paris, Fr. Bulletin de la Societe Chimique de France (

SOURCE:

AUTHOR(S):

**1967**), (4), 1117-25

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE:

Journal

```
LANGUAGE:
                          French
OTHER SOURCE(S):
                          CASREACT 67:117255
     16217-35-9P 16270-07-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and N.M.R. of)
RN
     16217-35-9 HCAPLUS
CN
     β-Alanine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)
i-PrNH-CH2-CH2-CO2H
RN
     16270-07-8 HCAPLUS
CN
     β-Alanine, N-propyl- (8CI, 9CI) (CA INDEX NAME)
n-PrNH-CH2-CH2-CO2H
     Et acrylate (I), diethyl fumarate (II), dimethyl maleate (III),
     MeCH: CHCO2Et (IV), and CH2: CMeCO2Me (V) are treated with PrNH2, iso-PrNH2,
     and Et2NH to give amino acids. Thus, a mixture of 0.05 mole I and 0.5 mole
     PrNH2 is kept 24 hrs. to give Et \beta-propylaminopropionate, b0.1
     32°. A mixture of 5.0 g. I and 1.5 g. PrNH2 is refluxed 10 hrs. to
     give diethyl \beta, \beta'-propyliminodipropionate, b0.4 98°.
     Also prepared are (reactants, product, b.p./mm., and m.p. given): iso-PrNH2
     and I, iso-PrNHCH2CH2CO2Et, 38°/0.4, -; iso-PrNH2 and I,
     iso-PrN(CH2CH2CO2Et)2, 92°/0.05, -; Et2NH and I, Et2NCH2CH2CO2Et,
     28°/0.08, -; PrNH2 and IV, MeCH(NHPr)CH2CO2Et, 36°/0.15, -;
     iso-PrNH2 and IV, Me(iso-PrNH)CHCH2CO2Et, 77°/11, -; PrNH2 and V,
     PrNHCH2CHMeCO2Me, 31°/0.15, -; iso-PrNH2 and V,
     iso-PrNHCH2CHMeCO2Me, 41°/0.1, -; PrNH2 and III,
     MeO2CCH2CH(NHPr)CO2Me, 65-6°/0.15, -; iso-PrNH2 and III,
     MeO2CCH2CH(NHPr-iso)CO2Me, 70°/0.3, -; Et2NH and III,
     MeO2CCH(NEt2)CH2CO2Me, 64°/0.3, -; PrNH2 and II,
     EtO2CCH (NHPr) CH2CO2Et, 91°/0.3, -; iso-PrNH2 and II,
     EtO2CCH(NHPr-iso)CH2CO2Et, 84°/0.4, -; Et2NH and II,
     {\tt EtO2CCH\,(NEt2)\,CH2CO2Et,\ 62^{\circ}/0.1,\ -;\ piperidine\ and\ III,\ di-Me}
     N, N-pentamethyleneaspartate, 98-101°/0.5, 44-4.5°;
     piperidine and III, Me \alpha-piperidino-\beta-
     piperidinocarbonylpropionate, -, 182-3° (decomposition). Also prepared
     are iso-PrNHCHMeCH2CO2Et-HCl, m. 118.5-19.5°, and iso -
     PrNHCH2CHMeCO2Me.HCl, m. 114-14.5°. The esters are hydrolyzed to
     give the following acids (m.p. given): PrNHCH2CH2CO2H, 150.5-1.5°;
     iso-PrNHCH2CH2CO2H, 165-6°; Et2NCH2CH2CO2H, 68-70°;
     Me (PrNH) CHCH2CO2H, 142-3°; Me (iso-PrNH) CHCH2CO2H, 165-6°:
     PrNHCH2CHMeCO2H, 136-7°; iso-PrNHCH2CHMeCO2H, 170.5-1.0°;
     MeO2C(PrNH)CHCH2CO2H, 151°; MeO2C(iso-PrNH)CHCH2CO2H,
     120.5-21°; EtO2C(PrNH)CHCH2CO2H, 165-7°;
     EtO2C (iso-PrNH) CHCH2CO2H, 94-5°, HO2CCH (NHPr-iso) CH2CO2H,
     170-2°. N.M.R. data are given for the prepared compds.
L38 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         1966:451518 HCAPLUS
DOCUMENT NUMBER:
                         65:51518
ORIGINAL REFERENCE NO.: 65:9660g-h,9661a
TITLE:
                         Systemic fungicides
INVENTOR(S):
                         Harnack, Willy; Schwarz, Justus
SOURCE:
                         3 pp.
DOCUMENT TYPE:
                         Patent
```

```
LANGUAGE:
```

Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DD 45884 19660205 DD 19641224 <-GB 1048507 GB

IT 542-53-0, Glycine, N-ethyl-, hydrochloride 627-01-0,
 Glycine, N-ethyl- 3182-82-9, Glycine, N-butyl-, hydrochloride
 3182-86-3, Glycine, N-isobutyl-, hydrochloride 3183-23-1
 , Glycine, N-isopropyl-, ethyl ester, hydrochloride 3338-22-5,
 Glycine, N-isopropyl-, hydrochloride 6939-13-5, Glycine,
 N-propyl-, hydrochloride
 (as fungicide)

RN 542-53-0 HCAPLUS

CN Glycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

EtNH-CH2-CO2H

## ● HCl

RN 627-01-0 HCAPLUS CN Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 $\mathtt{EtNH}-\mathtt{CH}_2-\mathtt{CO}_2\mathtt{H}$ 

RN 3182-82-9 HCAPLUS CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH2-CO2H

## ● HCl

RN 3182-86-3 HCAPLUS CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-BuNH-CH2-CO2H

# ● HCl

RN 3183-23-1 HCAPLUS
CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

Eto-C-CH2-NHPr-i

HCl

3338-22-5 HCAPLUS Glycine, N-(1-methylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H

● HCl

6939-13-5 HCAPLUS RN Glycine, N-propyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-PrNH-CH2-CO2H

### ● HCl

Glycine derivs. of the general formula RHNCH2CO2R' (R = H, Me, or Et) were systemic fungicides in vivo but not in vitro (spore germination test). Four young tomato plants with 4 or 5 leaves, in plastic pots were treated 2 times at 2-day intervals at the root stock with 3 ml. of test solution Two days later they were sprayed with a spore suspension of Phytophthora infestans, then placed in a moist chamber. After 4 days each plant was scored for fungus infestation on scale 0, 1, 2, 3, or 4 meaning no, mild, median, marked infestation, or plant destroyed, resp. Scores for water alone and for each fungicide in replicate rests were summed. The sum for water was set at 100, and the relative scores of fungicides recorded. 8 plants so treated with N-ethylglycine (I), N-ethylglycine-HCl (II), N-propylglycine-HCl (III), and N-2-hydroxyethylglycine (IV) in 0.5% solns., the relative infection scores were 0, 6, 10, 11, resp., and for 0.25% solns. 12, 10, 25, 20, resp. Eight plants sprayed sop. with solns. of II, III, and N-isopropylglycine-HCl were protected to a similar extent. Celery plants were protected against Septoria apii by root stock immersion in 0.5 and 0.25% solns. of the methyl esters and the methyl ester hydrochlorides of N-isopropylqlycine and N-allylglycine, the Et ester of N-allylqlycine, and N-butylqlycine, N-isobutylqlycine hydrochlorides. Areas of infection were usually smaller than in the controls. Development of reproductive structures is practically completely depressed.

L38 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:480952 HCAPLUS

DOCUMENT NUMBER:

63:80952

ORIGINAL REFERENCE NO.: 63:14970h,14971a-b

TITLE:

Monoalkylated glycine derivatives Hanke, H.

AUTHOR(S):

CORPORATE SOURCE: Univ. Jena, GA

```
SOURCE:
                         Pharmazeutische Zentralhalle fuer Deutschland (
                         1960), 99(June), 318-22
                         From: CZ 1963(26), 10820-1.
                         CODEN: PHZEAD; ISSN: 0369-9773
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         German
     542-53-0, Glycine, N-ethyl-, hydrochloride 627-01-0,
     Glycine, N-ethyl- 3182-81-8, Glycine, N-butyl- 3182-82-9
     , Glycine, N-butyl-, hydrochloride 3182-85-2, Glycine,
     N-isobutyl- 3182-86-3, Glycine, N-isobutyl-, hydrochloride
     3182-89-6, Glycine, N-isohexyl- 3182-90-9, Glycine,
     N-isohexyl-, hydrochloride 3183-21-9, Glycine, N-isopropyl-
     3183-22-0, Glycine, N-isopropyl-, ethyl ester 3183-23-1,
     Glycine, N-isopropyl-, ethyl ester, hydrochloride 3338-22-5,
     Glycine, N-isopropyl-, hydrochloride
        (preparation of)
RN
     542-53-0 HCAPLUS
CN
     Glycine, N-ethyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)
EtNH-CH2-CO2H
    ● HCl
RN
     627-01-0 HCAPLUS
     Glycine, N-ethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
EtNH-CH2-CO2H
     3182-81-8 HCAPLUS
RN
CN
     Glycine, N-butyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
n-BuNH-CH2-CO2H
RN
     3182-82-9 HCAPLUS
     Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)
n-BuNH-CH2-CO2H
     ● HCl
RN
     3182-85-2 HCAPLUS
CN
     Glycine, N-(2-methylpropyl) - (9CI) (CA INDEX NAME)
```

3182-86-3 HCAPLUS

i-BuNH-CH2-CO2H

RN

CN Glycine, N-(2-methylpropyl)-, hydrochloride (9CI) (CA INDEX NAME)

i-BuNH-CH2-CO2H

● HCl

RN 3182-89-6 HCAPLUS CN Glycine, N-isohexyl- (7CI, 8CI) (CA INDEX NAME)

 $Me_2CH-(CH_2)_3-NH-CH_2-CO_2H$ 

RN 3182-90-9 HCAPLUS CN Glycine, N-isohexyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

 $Me_2CH-(CH_2)_3-NH-CH_2-CO_2H$ 

● HCl

RN 3183-21-9 HCAPLUS CN Glycine, N-(1-methylethyl) - (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H

RN 3183-22-0 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

 $\begin{array}{c} \text{O} \\ || \\ \text{EtO-C-CH}_2\text{--NHPr-i} \end{array}$ 

RN 3183-23-1 HCAPLUS CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

O || EtO- C- CH2- NHPr-i

● HCl

RN 3338-22-5 HCAPLUS
CN Glycine, N-(1-methylethyl) -, hydrochloride (9CI) (CA INDEX NAME)

i-PrNH-CH2-CO2H

● HCl

Primary amine HCl salts with HCHO and KCN yield alkylamino-acetonitriles AΒ which can be hydrolyzed with alc. HCl to N-alkylglycines Et ester HCl salts. These treated with NH3-CHCl3 yield the free esters which are converted by acid saponification to the alkylglycine (Ia) and their HCl salts. Thus, to obtain N-ethylglycine (I), m. 180-2° (decomposition), I.HCl is treated with AgOH in water, the mixture filtered, the filtrate gassed with H2S, filtered, concentrated, and the residue dissolved in EtOH-Et2O. I.HCl m. 179-80°, is prepared by boiling 3 hrs. the Et ester (II) in 6N HCl, evaporating, and dissolving in EtOH-Et2O. To prepare II.HCl, m. 135°, HCHO, EtNH2.HCl, and KCN are allowed to react 30 min. in aqueous solution at 5° under CO2, the mixture kept several hrs., the nitrile formed extracted with Et20 (yield 90-100%), boiled 4 hrs. with ethanolic HCl, the NH4Cl filtered off and the filtrate concentrated; yield 90-100%. II, b16 58°, is obtained by 30-min. reaction of II.HCl and NH3-CHCl3 at 0  $^{\circ}$ filtering and distilling; yield 55-75%. Similarly were prepared the following Ia (alkyl, m.p., m.p. HCl salt, b.p. Et ester, and m.p. Et ester HCl salt given): isopropyl, 193-5° (decomposition), 202-3°, b2-3 32-5°, 113-15° (decomposition); allyl, 158-9° (decomposition), 167-9° (decomposition), b3 47°, 113-14° (decomposition) (EtOH); n-butyl, 190-1° (decomposition), 202-4°, b2-3 47-51°, 164-6°; isobutyl, 192-3° (decomposition), 210-12° (decomposition) or 221-222° (in sealed tube), b3 49-51°, 127-8.5° (decomposition); isohexyl, 194-5°, 186-7° b4 79°, 182-3°.

L38 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1963:435 HCAPLUS

DOCUMENT NUMBER:

58:435

ORIGINAL REFERENCE NO.: 58:63e
TITLE: Physics

Physicochemical analysis of isopropylamine-ethyl

monochloroacetate system

AUTHOR(S):

Bekturov, E. A.

SOURCE:

RN

Izvestiya Akademii Nauk Kazakhskoi SSR, Seriya

Khimicheskaya (1962), (1), 44-8 CODEN: IKAKAK; ISSN: 0002-3205

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

3183-22-0 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

 $\begin{array}{c} \texttt{O} \\ \parallel \\ \texttt{EtO-C-CH}_2 - \texttt{NHPr-i} \end{array}$ 

RN 3183-23-1 HCAPLUS

CN Glycine, N-(1-methylethyl)-, ethyl ester, hydrochloride (9CI) (CA INDEX

NAME)

EtO-C-CH2-NHPr-i

#### HCl

Measurement of viscosity, d., and conductivity of system Me2CHNH2 + CH2-ClCO2Et shows the formation of (Me2CHNH2CH2CO2Et)+.-Cl-, which then reacts with the 2nd mol. of amine to form Me2CHNHCH2CO2Et and Me2CHNH3Cl.

L38 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1956:52502 HCAPLUS

DOCUMENT NUMBER:

50:52502

ORIGINAL REFERENCE NO.: 50:10024h-i,10025a-d

TITLE:

The preparation of substituted hydrazines. III. A general method for preparing N-substituted glycines

AUTHOR(S):

Tien, Jack M.; Hunsberger, I. Moyer

CORPORATE SOURCE:

Antioch Coll., Yellow Springs, O.

SOURCE:

Journal of the American Chemical Society (1955

), 77, 6696-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal Unavailable

LANGUAGE:

56676-69-8, Glycine, N-hexyl-, hydrochloride

(preparation of)

56676-69-8 HCAPLUS RN

CNGlycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

 $Me^- (CH_2)_5 - NH^- CH_2 - CO_2H$ 

# HCl

cf. C.A. 50, 3431c. C6H13NH2 (0.765 g.) and 1.7 g. HOCH2CO2Et (62% pure) AB in 10 cc. glacial AcOH allowed to stand 2 hrs., hydrogenated with shaking 2 hrs. at room temperature and 3-4 atmospheric pressure over 0.1 g. 10% Pd-C, the

colorless filtrate neutralized with solid NaHCO3 and extracted with two 60-cc. portions Et20, the residue from the extract refluxed 10 min. with 5 cc. 10% aqueous NaOH, cooled, and acidified with 2-3 cc. concentrated HCl, and the precipitated

small, nearly white plates, m. 200-6°, heated with 25 cc. glacial AcOH on a steam bath, filtered hot, and cooled gave 0.4 g. N-hexylglycine (I) HCl salt, white flakes, m. 215-18°. The filtrate from the hydrogenation basified with dilute aqueous NaOH, refluxed cooled, acidified

excess concentrated HCl, and evaporated to dryness, and the residue extracted with hot

glacial AcOH gave I.HCl. C6H13NH2 and HOCH2CO2Et in 2:3 concentrated HCl-H2O gave only a very low yield of I.HCl; no I.HCl was detected from a hydrogenation in 6N HCl. PhNH2 (1.00 g.) in 5 cc. 95% EtOH and 1.70 g.

HOCH2CO2Et (62% pure) hydrogenated 2.5 hrs. and filtered, the catalyst washed with 10 cc. 95% EtOH, and the combined filtrate and washings diluted to the cloud point with H2O and cooled gave 1.06 g. N-phenylglycine Et ester (II), white plates, m. 57-8°; 2nd and 3rd crops, 0.41 and 0.17 g., resp. II (0.179 g.) refluxed 10 min. with 2 cc. concentrated HCl and

cc. H2O and evaporated to dryness in vacuo, the white residue dissolved with warming with 2 cc. concentrated HCl on the steam bath, and the solution cooled gave

0.116 g. N-phenylglycine-HCl salt, m. 172-4°; 2nd crop, 0.041 g. Com. N-phenylglycine (0.1 g.), yellow powder, and 0.1 g. NaCl dissolved at about 70° in 5 cc. H2O, and the solution cooled deposited after about 2 min. large pale-yellow needles; a similar recrystn. in the presence of 0.5 cc. AcOH gave colorless crystals, m. 126-7°; the free base dissolved with heating in concentrated HCl on the steam bath, decolorized, and cooled deposited the HCl salt, colorless transparent plates, m. 168-73°; turned lemon-yellow after several days.

L38 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1956:12242 HCAPLUS

DOCUMENT NUMBER: 50:12242

ORIGINAL REFERENCE NO.: 50:2534d-i,2535a-i,2536a-b

TITLE: The preparation of substituted hydrazines. I.

Alkylhydrazines via alkylsydnones

AUTHOR(S): Fugger, Joseph; Tien, Jack M.; Hunsberger, I. Moyer

CORPORATE SOURCE: Antioch Coll., Yellow Springs, O.

SOURCE: Journal of the American Chemical Society (1955

), 77, 1843-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 50:12242

IT 3182-82-9, Glycine, N-butyl-, hydrochloride 56676-69-8,

Glycine, N-hexyl-, hydrochloride

(preparation of) 3182-82-9 HCAPLUS

CN Glycine, N-butyl-, hydrochloride (7CI, 8CI, 9CI) (CA INDEX NAME)

n-BuNH-CH2-CO2H

RN

● HCl

RN 56676-69-8 HCAPLUS

CN Glycine, N-hexyl-, hydrochloride (9CI) (CA INDEX NAME)

 $Me^{-(CH_2)}_{5}-NH^{-CH_2-CO_2H}$ 

● HCl

AB The conversion of an alkylamine to an alkylhydrazine via the corresponding N-alkylglycine, N-nitroso-N-alkylglycine, and N-alkylsydnone is shown to constitute an acceptable preparative method in the cases of PhCH2NHNH2

(I), BuNHNH2 (II), and C6H13NHNH2 (III). The infrared spectra of N-benzylsydnone (IV), N-butylsydnone (V), and N-hexylsydnone (VI) are presented. ClCH2CO2Et (122 g.) and 214 g. PhCH2NH2 in 1 l. C6H6 refluxed 5 hrs. with stirring, the mixture filtered, the filtrate distilled to leave 154 g. PhCH2NHCH2CO2Et, yellow oil, the residue filtered, the crude ester added dropwise with stirring during 15 min. to 63.6 g. NaOH in 300 cc. H2O, the yellow solution refluxed 45 min. washed with Et2O, and acidified with concentrated HCl to pH 2, the resulting white suspension of PhCH2NHCH2CO2H treated at 0° with stirring during 0.5 hr. with 55.2 g. NaNO2 in 100 cc. cold H2O, the mixture stirred 2 hrs., brought to pH 2 with concentrated HCl, refrigerated 1 hr., and filtered, and the filter residue dried in vacuo over KOH yielded 139 g. crude PhCH2N(NO)CH2CO2H (VII). The VII heated 5 hrs. with stirring on the steam bath with 685 cc. Ac20, the resulting dark red solution filtered, and the filtrate evaporated in vacuo yielded 115 g. crude IV, red-brown oil, which solidified in an ice bath on scratching. The crude IV heated 4.5 hrs. on a steam bath with 1 l. 1:1HCl, the red solution filtered, the clear filtrate concentrated to less than

100

cc. and filtered, and the residual crude I.HCl (56.8 g.) recrystd. twice from boiling EtOH yielded 14.6 g. pure I.HCl, m. 108-10.5°; and from mother liquor an addnl. 6.1 g. I.HCl. BrCH2CO2Et (68 cc.) in 100 cc. C6H6 added portionwise with swirling and cooling to 120 cc. BuNH2 in 300 cc., the mixture refluxed 2 hrs. on a steam bath, cooled, and filtered, the residual HBr salt (59 g.) washed with 80 cc. C6H6, the combined filtrate and washing concentrated in vacuo until white fumes appeared, the residue refluxed 25 min. with 28 g. NaOH in 120 cc. H2O, the cooled alkaline solution extracted with Et2O, the aqueous layer acidified with cooling to pH 2 with concentrated

HCl, and the mixture refrigerated and concentrated consecutively yielded 68.9 g.

crude BuNHCH2CO2H.HCl (VIII).HCl, snow-white needles and plates. Crude VIII.HCl (1 g.) in 10 cc. concentrated HCl warmed slightly on the steam bath and

filtered, the filtrate refrigerated, and this process repeated 3 times gave pure VIII.HCl, m. 204-5°. C6H13NH2 and BrCH2CO2Et gave in exactly the same manner crude C6H13NHCH2CO2H.HCl (IX.HCl); the alkaline solution

of the IX.HCl swirled with cooling with 90 cc. concentrated HCl and 100 g. chopped ice precipitated immediately 81.0 g. IX.HCl, tiny yellowish white flakes;

refrigeration of the mother liquor gave an addnl. 4.8 g. IX.HCl. Crude IX.HCl (1 g.) in 10 cc. H2O treated with 1 cc. concentrated HCl, and the resulting precipitate treated 3 times in the same manner gave pure IX.HCl, snow-white flakes, m. 210-17°. Crude IX.HCl (1 g.) recrystd. from 20 cc. 1:1 MeOH-Me2CO or 40 cc. glacial AcOH gave the pure salt. VIII.HCl (78.0 g.) in 300 cc. H2O treated during 0.5 hr. at -4 to -5° with 37.5 g. NaNO2 in 100 cc. H2O, the mixture stirred 2 hrs., the oily bottom layer drawn off and dissolved in Et2O, and the solution filtered, dried, and evaporated gave 62.0 g. crude BuN(NO)CH2CO2H (X), yellow granular powder. Crude X (8.0 g.) crystallized from a small amount Et2O gave 4.53 g. nearly white

granular solid, m. 60-2°, which recrystd. from aqueous EtOH or Et2O-petr. ether gave pure X, long snow-white flakes, m. 61-2°. An alkaline solution of IX prepared from 0.60 mole BrCH2CO2Et, cooled, treated with

stirring with 49.7 g. NaNO2 in 100 cc. H2O in 1 portion followed dropwise during 1.25 hrs. by 90 cc. concentrated HCl diluted with 50 g. ice, stirred 1 hr.,

and adjusted with concentrated HCl to pH 2.0, the resulting brown oily top layer

of crude C6H13N(NO)CH2CO2H (XI), (74.8 g.) allowed to stand, and the solidified yellow granular powder recrystd. from Et2O and then aqueous EtOH or petr. ether-Et2O gave pure XI, long white flakes, m. 79-80°. Crude X (40 g.) in 236 cc. Ac2O heated 3 hrs. on the steam bath, the mixture kept 1 day at room temperature, and the excess Ac2O distilled off gave 33 g. crude V; an

8-g. sample distilled yielded 4.5 g. pure V, pale yellow oil, b2 165-7°. X (0.362 mole) heated 3 hrs. with only 1.09 moles Ac20 gave nearly identical results. Crude yellow-white XI prepared from 0.20 mole BrCH2CO2Et dissolved in Et2O, the extract dried over Na2SO4, treated with 190 cc. Ac2O, kept 1 day at room temperature, and evaporated on the steam bath.

the residual oil refluxed 3 hrs., the excess Ac2O removed in vacuo, and the clear brown oil dried in vacuo over KOH and P2O5 yielded 23 g. crude VI, which on distillation yielded 18 g. pure VI, b0.43 170-6° (redistd., b0.09 141-3°). XI (0.334 mole) dissolved in 1.14 moles warm AcOH, and the brown solution heated 2 hrs. on the steam bath after standing overnight yielded 93% VI. Crude V (40.5 g.) mixed with 80 cc. concentrated

the mixture heated 2 hrs. on the steam bath, cooled to room temperature, treated

HCl,

with 20 cc. concentrated HCl, refrigerated overnight, treated with dry HCl to beginning crystallization, refrigerated again, and filtered, the residue washed with 1:1 MeOH-Et2O to yield 22 g. nearly white transparent needles, the filtrate decolorized with Norit A, saturated below 0° with dry HCl, refrigerated several days, neutralized with solid Na2CO3, and extracted with Et2O, a part of the extract treated with dry HCl, and the white precipitate filtered

off gave II.HCl; the remainder of the extract treated in EtoH with  $(CO2H)\ 2$  yielded the oxalate of II. Distilled V  $(4.4\ g.)$  heated 2.5 hrs. with concentrated

HCl, the yellow solution treated after 2 hrs. with an addnl. 10 cc. HCl, and the solution cooled and saturated with dry HCl yielded 3.1 g. II.HCl, thin white

plates, m. 149-54°. II.HCl (3.0 g.) treated with 15 cc. 25% aqueous Na2CO3, the alkaline mixture extracted with Et2O, and the extract distilled gave 1.0 g. V,

colorless liquid with an amine odor, b20 82-5°. Crude VI.HCl (40.7 g.) and 80 cc. concentrated HCl heated 2 hrs. on the steam bath, the mixture treated with an addnl. 30 cc. HCl and refrigerated, the dark brown cake dissolved in about 150 cc. H2O, and the solution heated a few min. on the steam bath with about 5 g. Norit, filtered hot, and cooled deposited 19.8 g. III.HCl, fine transparent needles; the mother liquor treated with (CO2H)2 in EtOH gave 18.0 g. III oxalate. The alkaline solution of the Na salt of IX from 0.60 mole BrCH2CO2Et treated below 0° with 37.2 g. NaNO2 in 120 cc. H2O in 1 portion, the mixture allowed to stand 0.5 hr., treated with 100 cc. concentrated HCl containing 50 g. crushed ice, stirred 1 hr., and extracted

with Et20, and the Et20 evaporated gave a residue of 88.7 g. XI. XI (83.7 g.) heated 2 hrs. on the steam bath with 126 cc. Ac20, the excess Ac20 removed gave 81.5 g. crude VI. Crude VI (64 g.) heated 2 hrs. on a steam bath with 110 cc. concentrated HCl, cooled, neutralized with 25% aqueous NaOH, saturated with

K2CO3, and extracted 8 times with Et2O, the extract dried with K2CO, and added to

76 g. (CO2H)2 in 400 cc. 95% EtOH, the mixture allowed to stand overnight, and the yellowish solid filtered off and dried yielded 55.5 g. crude III.(CO2H)2. Crude III.(CO2H)2 (1.0 g.) recrystd. from 25 cc. hot 9:1 MeOH-EtOH yielded 410 mg. fluffy flakes, m. 171-2°; a 94-mg. sample in 5 cc. hot MeOH evaporated slowly at room temperature yielded 64 mg. large white

needles, m. 173-3.5°; this material dissolved in 5 cc. hot 4; 1 MeOH-EtOH, the solution filtered, and the filtrate poured into a sintered glass funnel gave 26 mg. pure III.(CO2H)2, transparent needles, m. 174.5-5.5°. II.HCl dissolved in 150-200 cc. H2O, neutralized with 30% aqueous NaOH in portions, saturated with solid K2CO3, and extracted with Et2O, the

extract dried over K2CO3 and added to 54 g. (CO2H)2 in 320 cc. 95% EtOH, the mixture allowed to stand overnight and filtered to give 18.5 g. crude salt, the mother liquor of the original II.HCl treated in the same manner to give an addnl. 6.3 g. oxalate, and the solid material combined gave 24.8 g. crude II.(CO2H)2. Crude II.(CO2H)2 (1 g.) recrystd. from 60 cc. hot 9:1 MeOH-EtOH yielded 420 mg. pure material, fine snow white needles; a sample (180 mg.) recrystd. from 20 cc. of the same solvent yielded 144 mg. pure material, white needles, m. 164-5°.

#### => FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 08:19:19 ON 03 JUN 2004 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 28, 2004 (20040528/UP).

=>

**ચ**ા છે.